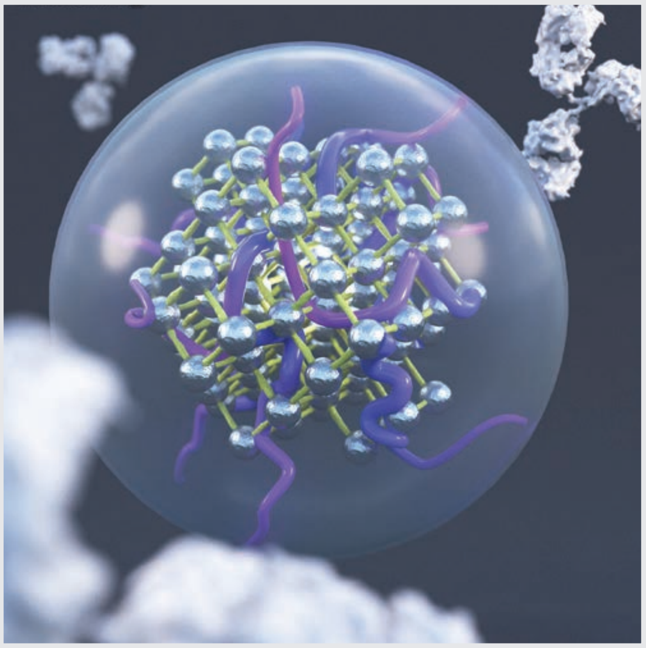
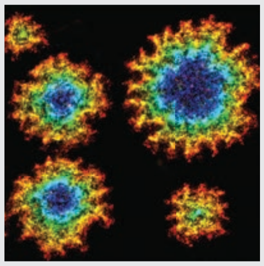
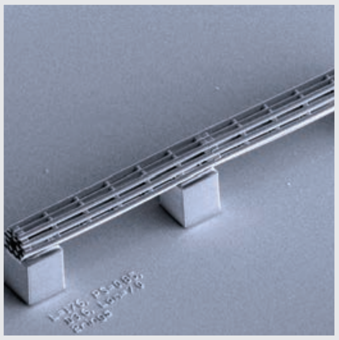
CENTER FOR NANOSCIENCE
ANNUAL REPORT 2019







CeNS
Center for NanoScience | LMU

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2019 was another successful year for CeNS in terms of its main goals – research cooperation, interdisciplinary training, and technology transfer. We had a year of intense discussions about where CeNS will be going in the future – especially with regard to its very successful daughters that emerged from the NanoSystems Initiative Munich, namely the MCQST and the E-conversion cluster. We concluded that we will stay close to our roots, continuing CeNS' special expertise in enabling networking between disciplines and being the fertile ground for future topics in nanoscience and for innovative start-ups. We have seen how the great community spirit of CeNS leads the way: Biophysics moves towards Physics of Living Systems; CeNS was the thinktank to develop the cross-disciplinary Engineering Life initiative at the LMU, and the Emergence of Life network initiatives were started within CeNS, now connecting Nanoscience even to molecular astrophysics with the Origins Cluster. Being curious and opening new fields between the disciplines will be the seed for the new hot topics for the next rounds of Excellence and European-wide initiatives.

The CeNS community keeps growing and we are very happy to welcome our new members at the Physics Department Stefan Maier, Emiliano Cortés, and Andreas Tittl. With the new members Johannes Stigler from the Gene Center, Hannes Mutschler at the MPI of Biochemistry and Kurt Schmoller at the Helmholtz Center Munich, new, valuable links are being created.

A very special anniversary was celebrated last year: In September, nearly 200 biophysicists from all over the world came together for the festive symposium in honor of Hermann Gaub. Hermann is one of the co-founders of CeNS, and we would like to express our sincere gratitude to him for his immense contributions to shaping CeNS over the years with his ideas and both as CeNS spokesman and board member.

A particular highlight of the CeNS 2019 calendar was the four-day International Physics Of Living Systems (iPoLS) Meeting organized by Don Lamb and Philip Tinnefeld in Munich, with CeNS and SFB1032 acting as hosts. The conference attracted more than 250 participants and speakers from all over the world, endorsing the international standing of Munich in the field of biophysics.

The annual workshop in Venice was co-organized by CeNS and the CRC235 "Emergence of Life" this time. The theme of the meeting was *Evolving Nanosciences*, bridging Origin-of-life research with nanoscientific topics. The Junior NanoScience Network 2019 connected our PhD students with the nanoscience done at the UCSB in Santa Barbara. The visit back in Munich and Venice was a highlight long remembered by the participating labs, confirming the Venice workshop is a unique cross-disciplinary format which connects many different topics.

CeNS has again been successful in translating new ideas into the real world: MassivePhotonics, a new start-up from the Jungmann lab, brings ready-to-use labeling reagents for DNA-PAINT to the user, to transform the super-resolution microscopy market. For the Nano Innovation Award 2019, excellent proposals across the entire state of Bavaria were submitted and two innovative theses were honored by CeNS together with the spin-offs attocube, ibidi, Nanion and NanoTemper. The award also serves as an encouragement for young researchers who are on the verge of transferring their findings into a start-up.

We hope you will enjoy reading the CeNS annual report with all of last year's activities and of course the science that drives us. Last but not least, on behalf of all CeNS members, we would like to thank the CeNS management team Susanne Hennig, Claudia Leonhardt and Marilena Pinto for their continuous support and commitment!

Prof. Dieter Braun
Spokesman of the Scientific Board of CeNS

NEW MEMBERS

PROF. EMILIANO CORTÉS

LMU Munich

Emiliano Cortés holds a W2 tenure-track professorship at the Physics Department at LMU Munich and is the academic lead of the Plasmonic Chemistry Group. He is also a visiting researcher at the Chemistry Department, University College London, UK, and at the Physics Department, Imperial College London, UK. His research interests lie at the interface between chemistry and physics, and focus on the development of novel nanomaterials and techniques, specifically for applications in energy conversion.

Emiliano studied chemistry at the National University of La Plata in Argentina. He was one of the founders of Nanodetection, a start-up company based on plasmonic sensing. He was also a Marie-Skłodowska-Curie research fellow at Imperial College London. In 2018, he was awarded with the ERC Starting Grant from the European Commission for his project CATALIGHT.

PROF. STEFAN MAIER

LMU Munich

Stefan Maier holds the Chair in Hybrid Nanosystems in the Faculty of Physics, established 2018. He also has a part-time position at Imperial College London, where he holds the Lee-Lucas Chair in Experimental Physics. His research interests are in fundamental and applied plasmonics, nanophotonics, energy conversion, and optoelectronics.

A graduate from Caltech, Stefan was awarded the Sackler Prize in the Physical Sciences and the Paterson Medal of the Institute of Physics. He held a Royal Society Wolfson Research Merit Award and is a fellow of the IoP and the Optical Society of America. He further is an ISI Highly Cited Researcher in 2018 and 2019.

DR. HANNES MUTSCHLER

MPI of Biochemistry

Hannes Mutschler is an independent research group leader at the Max Planck Institute of Biochemistry in Martinsried. He received an M.Sc. (Diplom) in biophysics from the Humboldt University of Berlin and a Ph.D. on programmed cell-death in bacteria from the Max Planck Institute of Medical Research in Heidelberg, Germany. For his postdoc on origins of life research, he joined Phil Holliger's lab at the MRC Laboratory of Molecular Biology in Cambridge, UK where he studied RNA catalysis in frozen environments. In 2016, he started his own lab at the MPI of Biochemistry as part of the MaxSynBio consortium. His current research interests include bottom-up synthetic biology including cell-free protein synthesis as well as RNA catalysis and replication. In 2018, he was awarded an ERC Starting grant.

DR. KURT SCHMOLLER

Helmholtz Zentrum München

Kurt Schmoller is an Independent group leader at the Institute of Functional Epigenetics at the Helmholtz Zentrum Munich. He studied biophysics at the TU München, where he also did his PhD with Andreas Bausch, working on the dynamics and mechanics of reconstituted actin systems. After graduating in 2012, he joined the lab of Jan Skotheim at Stanford University, where his interests shifted to the budding yeast cell cycle. In 2017, he started his own lab at the Helmholtz Zentrum. His interdisciplinary group uses a wide range of methods, ranging from yeast genetics to live-cell imaging and mathematical modelling, to study how cells coordinate protein and organelle homeostasis with cell size and growth. In 2019, he was awarded an HFSP Career Development Award.

PROF. JOHANNES STIGLER

LMU Munich

Johannes Stigler holds a W2 tenure-track professorship at the Gene Center at LMU Munich. After studying physics at the LMU, he did his Ph.D. with Matthias Rief at the TU Munich. In 2013, he joined the lab of Eric Greene at Columbia University for a postdoctoral stay with a Feodor Lynen Postdoctoral Fellowship. In 2017, he returned to Germany and started his own lab at the Gene Center as an independent Emmy Noether group leader. His lab uses biophysical single molecule techniques to determine the processes that lead to the three-dimensional folding of chromosomes.

DR. ANDREAS TITTL

LMU Munich

Andreas Tittl is subgroup leader for mid-infrared nanophotonics at the Chair in Hybrid Nanosystems (Prof. Maier) at LMU. He received his Ph.D. in physics from the University of Stuttgart, Germany, in 2015, focusing on the development of optical sensors for the detection of gases and catalytic reactions. Afterwards, he became a Marie-Curie-funded EPFL Fellow in Prof. Altug's lab at Ecole Polytechnique Fédérale de Lausanne, Switzerland, working on mid-infrared spectroscopic biosensing. His current research targets the design and implementation of novel surface-enhanced nanophotonic approaches for understanding complex biological systems, where he has recently pioneered the use of all-dielectric metasurfaces in IR biochemical spectroscopy. Dr. Tittl has received several awards for his work, including the VDI Young Researcher Award Nanotechnology, the Young Investigator Award „Green Photonics", and the Jeffrey Hubbell and Melody Swartz Young Bioengineer Award.

MEMBERS' NEWS

Prof. Erwin Frey (LMU) held the Kavli Chair 2019 at the Kavli Institute of Nanoscience Delft.

Prof. Chase Broedersz (LMU) accepted a position as full professor at the Vrije Universiteit Amsterdam.

Dr. Ulrich Lächelt (LMU) won the Galenus Technology Prize 2019.

Dr. Hanna Engelke (LMU) received a call for a professorship from the Karl-Franzens-Universität Graz.

Prof. Jan Lipfert (LMU) won the teaching prize of the Physics Department ("Goldener Sommerfeld").

Prof. Eva Weig (University of Konstanz) received a call for the Chair for Nano and Quantum Sensors (W3) at TU Munich.

Prof. Stefan Maier (LMU) received the 2020 ACS Nano Lectureship.

Prof. Thomas Weitz (LMU) accepted a position as W3 at the Faculty of Physics, Georg-August-University Göttingen.

Prof. Petra Schwille (MPI of Biochemistry) received the Bavarian Maximilian Order for Science and Art.

Dr. Christoph Westerhausen (University of Augsburg) accepted position as permanent research group leader at the University of Augsburg, Medicine Department.

CENS PUBLICATION AWARDS 2019

On November 22, the winners of the 2019 CeNS Publication Awards were announced to the CeNS members and students after the CeNS Annual Assembly. The awards recognized successful cooperation projects within CeNS as well as outstanding research by individual research groups from CeNS. Another prize category is specifically devoted to junior scientiest within CeNS. As is tradition, the winners were celebrated at the annual CeNS "Get-Together" event in the Café an der Universität.

Best Interdisciplinary Publications:

- D. B. Brückner, A. Fink, C. Schreiber, P. J. F. Röttgermann, **J. O. Rädler** and **C. P. Broedersz**; Nature Physics (see page 23)
- M. Morasch, J. Liu, C. F. Dirscherl, A. Ianeselli, A. Kühnlein, K. Le Vay, P. Schwintek, S. Islam, M. K. Corpinot, B. Scheu, D. B. Dingwell, P. Schwille, **H. Mutschler,** M. W. Powner, **C. B. Mast** and **D. Braun**; Nature Chemistry (see page 28)
- B. Rogez, L. Würthner, A. B. Petrova, F. B. Zierhut, D. Saczko-Brack, M.-A. Huergo, C. Batters, **E. Frey** and **C. Veigel**: Nature Comm. (see page 21)
- J. Stein, F. Stehr, P. Schueler, P. Blumhardt, F. Schueder, J. Mücksch, **R. Jungmann** and **P. Schwille**: Nano Letters (see page 25)

Scientific Breakthrough:

- M. Förg, L. Colombier, R. K. Patel, J. Lindlau, A. D. Mohite, H. Yamaguchi, M. M. Glazov, D. Hunger and **A. Högele**; Nature Comm. (see page 29)
- J. Lenz, F. del Giudice, F. R. Geisenhof, F. Winterer and **R. T. Weitz**; Nature Nanotechnology (see page 22)
- A. Löf, P. U. Walker, S. M. Sedlak, S. Gruber, T. Obser, M. A. Brehm, **M. Benoit and J. Lipfert:** PNAS (see page 52)

Best Junior Scientist Publications:

- **P. Rovó**, C. A. Smith, D. Gauto, B. L. de Groot, P. Schanda and R. Linser; Journal of the American Chemical Society (see page 40)
- A. Zimpel, N. Al Danaf, B. Steinborn, J. Kuhn, M. Höhn, T. Bauer, P. Hirschle, W. Schrimpf, **H. Engelke, E. Wagner,** M. Barz, **D. C. Lamb, U. Lächelt** and **S. Wuttke**, ACS Nano (see page 42)
- H. Huang, Y. Li, Y. Tong, E.-P. Yao, M. W. Feil, A. F. Richter, M. Döblinger, **A. L. Rogach, J. Feldmann** and **L. Polavarapu;** Angewandte Chemie International Edition (2019)

- www.cens.de/research/cens-publication-award

Left: The CeNS Get-Together in the "CadU". **Right:** Winners in the category "Scientific Breakthrough: Martin Benoit, Achim Löf, Sophia Gruber and Steffen Sedlak (from left).

X-RAY VISION ON NANOPARTICLES AND A HALL OF MIRRORS FOR NANOMICROSCOPY - NANO INNOVATION AWARD 2019

NANO INNOVATION
AWARD 2019

On July 19, the Nano Innovation Award 2019 was presented at CeNS at LMU Munich. Two young researchers from Bayreuth and Munich received the award for promising results as part of their master's or doctoral thesis. The Nano Innovation Award focuses specifically on innovative work with promising application potential in technology or medicine. The Bavarian-wide prize is endowed with €9,000 and is awarded annually by a jury of experts from science and business.

A better understanding of nanoparticles' interactions

Nanoparticles finely distributed in solution are nowadays widely applied in industrial applications, e.g., as catalysts, as UV-filter in cosmetic products, in sunscreen, or as drug vehicles in biomedical applications. Since experimental access has been very difficult, only little is known so far about the properties and the structure of the interface between nanoparticles and surrounding water molecules. In her Master's thesis, Sabrina Thomä from the University of Bayreuth succeeded in investigating the arrangement of water molecules in the vicinity of iron oxide nanoparticles with high-energy X-rays. For this work, she was awarded the Nano Innovation Award in the master's category, worth €3,000. "I was surprised about the detailed insight into the hydration shells and that the water structure around 7 nm colloidal particles does not differ significantly from the structure at bulk surfaces", says Sabrina Thomä, who is currently a PhD student in Chemistry in the group of Mirijam Zobel at the University of Bayreuth.

One million photons – and only one is missing

The Nano Innovation Award for the best doctoral thesis, endowed with €6,000, went to Thomas Hümmer from the group of Prof. Theodor Hänsch at LMU Munich and MPI for Quantum Optics. In his work, Thomas Hümmer developed a new kind of highly sensitive microscope to explore optical properties of nano-objects. Using two opposing mirrors, light is reflected back and forth hundreds of thousands of times. If a nanoparticle is placed between the mirrors, its interaction with light will be strongly enhanced, allowing detection of light absorption as weak as one photon in a million. As one of the mirrors is only the size of a human hair, a scanning microscope can be built that

From left to right: Charles Heffner (NanoTemper), Prof. Alexander Högele (Jury Nano Innovation Award), Dr. Susanne Hennig (CeNS), Awardee Thomas Hümmer, Awardee Sabrina Thomä, Prof. Philip Tinnefeld (CeNS Board and Jury Nano Innovation Award), Dr. Axel Thierauf (Jury Nano Innovation Award).

enables highly sensitive imaging and spectroscopy of tiny structures for material research, nanotechnology, and life sciences.
Thomas Hümmer has already developed a portable, fully functional prototype of this new microscope. Currently, he works on commercializing his findings by starting his own company Qlibri.

An institution boosting careers

The Center for NanoScience awards the Nano Innovation Award together with four companies that are spin-offs from CeNS: attocube systems, ibidi, Nanion Technologies and NanoTemper Technologies. "With this award, we want to emphasize the importance of fundamental research as a basis for industrial applications. At the same time, we would like to encourage researchers to start their own companies with their expertise and ideas, thus making their knowledge applicable for many," said Dr. Philipp Baaske, CEO and founder of NanoTemper Technologies and member of the jury.

- www.cens.de/research/nano-innovation-award

CENS TRAVEL AWARDS

In 2019, eight CeNS PhD students and three postdocs won CeNS travel awards to present their work at international conferences and workshops. The recipients of the awards came from different CeNS groups from the Department of Chemistry, and the Department of Physics. The CeNS travel award comes with up to €1,500 for travel costs.

- **Kira Bartnik** (AG Lamb), Talk at the Biophysical Society Annual Meeting 2020, San Diego

- **Magnus Bauer** (AG Gaub), Talk at the Molecule Biophysics meeting at École de Physique, Les Houches

- **Dr. Richard Ciesielski** (AG Hartschuh), Poster at the 11th International Conference on Hybrid & Organic Photovoltaics (HOPV19), Rom

- **Nader Danaf** (AG Lamb), Poster at the MAF Conference in La Jolla, San Diego

- **Jan Felber** (AG Thorn-Seshold)**,** Poster at the 3rd Symposium of the SPP1710, San Feliu/Spain

- **Dr. Viktorija Glembockyte** (AG Tinnefeld), Talk at "Methods and Applications of Fluorescence", San Diego

- **Carola Lampe** (AG Urban), Talk at the 2019 MRS Spring Meeting, Phoenix

- **Joris Messelink** (AG Broedersz), Poster at qBio, San Francisco

- **Stefanie Pritzl** (AG Lohmüller), Talk at the 2019 MRS Fall Meeting, Boston

- **Steffen Sedlak** (AG Gaub), Poster/Talk at the MechanoChemBio 2019, Montreal

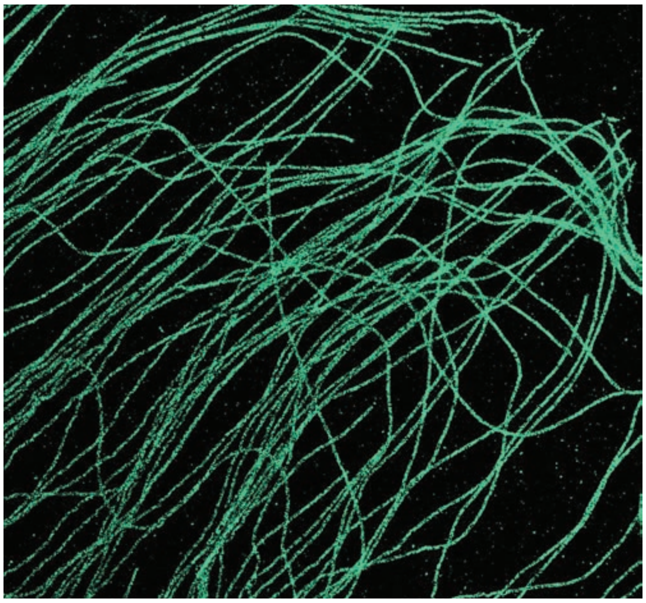
- **Dr. Florian Selbach** (AG Tinnefeld), Talk at the ICES2019, Ontario
- www.cens.de/research/travel-award

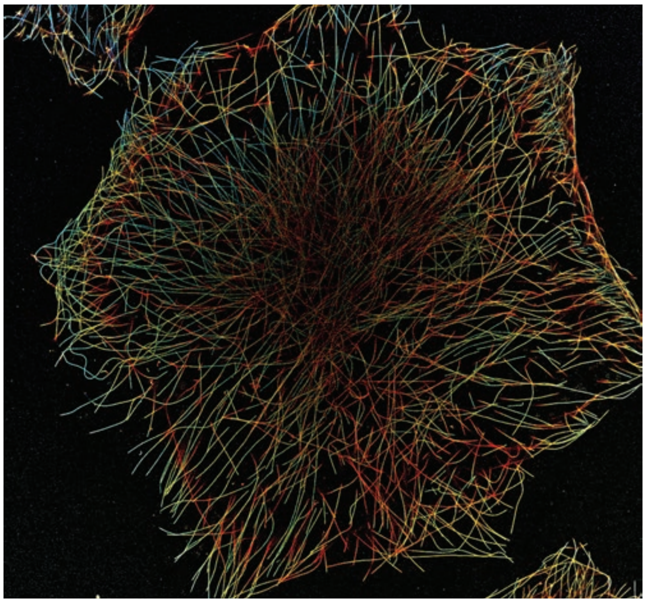
MASSIVE PHOTONICS

MASSIVE PHOTONICS - LABELING REAGENTS FOR DNA-PAINT

The new start-up Massive Photonics aims to bring ready-to-use labeling reagents for DNA-PAINT to the user and is geared-up to transform the super-resolution microscopy market. Ralf Jungmann's group at the MPI of Biochemistry and LMU Munich and colleagues have developed DNA-PAINT with the goal to simplify super-resolution microscopy and lower the entry barrier for novice users. The technique uses short, dye-labeled DNA strands that transiently interact with their target-bound complements in order to create the necessary "blinking" for super-resolution.
The team has developed DNA-conjugated labeling reagents over the years to efficiently target protein targets in cells. "There has been a growing interest in the community to get easy access to DNA-conjugated labeling reagents to perform DNA-PAINT experiments", says Sebastian Strauss, co-founder and CTO of Massive Photonics. We are excited to now make the step into the commercial market with Massive Photonics and develop novel products and assays with our customers in the future", says Jungmann, who is the third co-founder of the startup.
Source: MPI of Biochemistry Press Release

- www.massive-photonics.com





CENS/CRC235 VENICE WORKSHOP

"Evolving Nanosciences" – this was the motto of the 2019 workshop at Venice International University, jointly organized by CeNS and the Collaborative Research Centre 235 "Emergence of Life". CeNS and CRC235 researchers and invited speakers gathered on the island of San Servolo for a varied program. Once again, the program committee had drawn up an impressive schedule with renowned speakers: Job Bokhoeven, Tom de Greef, Zvonimir Dogic, Andrew D. Griffiths, Rupert Huber, Dahlia Klein, Sergei Maslov, Wolfgang Parak, Francesco Ricci, Carmen Rubio Verdú, David Rueda, Nita Sahai, Markus Sauer, Christoph Schmidt, Jon Stewart, Christoph Weber, Paul S. Weiss, Alex Weber-Bargioni, Jerome Wenger, Wesley Wong, Ursula Wurstbauer, Tetsuya Yomo, and Gil Westmeyer. In addition, five researchers from CeNS presented their research. The talks covered a wide range of topics, from origin of life research and single-molecule studies to DNAbased nanodevices and nanoelectronics. Moreover, CeNS and CRC235 graduate students as well as JNN participants from UC Santa Barbara presented and held a lively discussion of their latest results during the two outdoor poster sessions. As every year, the island San Servolo captivated the workshop participants with its charming and relaxed atmosphere.

■ www.cens.de/calendar/workshops-events/venice-2019/

PHYSICS OF LIVING SYSTEMS MEETING 2019

The Physics of Living Systems (PoLS) Student Research Network is an international network of graduate students and educators. The program targets synergy of theoretical and experimental research at the interface between biology and physics. The 2019 international PoLS meeting was hosted by CeNS and SFB1032 and was attended by over 270 participants from 20 institutions. It took place at the MPI of Biochemistry from July 8 to 11. The organizers Prof. Don Lamb and Prof. Philip Tinnefeld were supported by the management teams of CeNS and the SFB1032. About 70 talks by faculty and graduate students gave a remarkable insight into the world of physics of living systems. In addition, about 110 poster presenters got the chance to present their work in a flash talk before the poster sessions. Moreover, in an "unconference" format group discussions on previously

proposed topics such as “Engaging with the public”, “From PhD to tenure”, or “Research and ethics” were enabled. To enhance networking between participants, an interactive conference app was used for the meeting. The social program included a conference dinner and different activities, such as a roof climb on the glass roof of the famous Olympic stadium.

■ www.cens.de/calendar/workshops-events/ipols-2019/

ANNIVERSARY WORKSHOPS

On September 6th and 7th, nearly 200 biophysicists from all over the world came together for the festive symposium in honor of Hermann Gaub, who holds the LMU chair for biophysics and molecular materials and is one of the co-founders of the Center for NanoScience. *Stretching the boundaries of physics, one molecule at a time* was organized by CeNS, Prof. Matthias Rief and the members of the biophysics chair (Sylvia Kreuzer, Jan Lipfert and Martin Benoit). Biophysicists from all parts of the world met to exchange and lively discuss outstanding scientific results and developments in nano biophysics.

■ www.biophysik.physik.uni-muenchen.de/news

Another co-founder of CeNS was honored in September, too: The symposium *Many-body physics with ultracold atoms and beyond* on September 5th and 6th was organized by CeNS member Matthias Punk and others to celebrate Wilhelm Zwerger, chair of theoretical physics at TU Munich. The aim of the workshop was to bring together leading researchers in the fields of quantum many-particle systems, such as ultracold quantum gases, optomechanics, and cavity QED systems in nanostructures, to explore new frontiers and to identify open questions and challenges.

FROM THE IDEA TO A SUCCESSFUL PATENT

The right IP strategy plays an important role in the commercial success of a nanotechnology-based invention. On April 10 and 11, CeNS and the Nanotechnology Cluster organized a joint workshop on the topic, supported by patent attorney SR Huebner. More than 50 participants took part in the event. The focus of the first workshop day was on the experience reports of representatives from SMEs and start-up companies: In interesting lectures, Dr. Ruth Houbertz, Multiphoton Optics GmbH, Dr. Valentin Kahl from ibidi GmbH and Dr. Heinrich Grabmayr from pre-startup DEOXY Technologies, informed about the challenges of patenting. In addition, Dr. Huebner gave an overview of measures to protect nanotech inventions and Jens Weckesser spoke about the patenting process at the European Patent Office (EPO). The second day was dedicated to a mock trial, in which the participants worked on a real case in the roles of patent owner, patent infringer and patent judge. The actual mock trial was lively and full of discussions – a true learning experience for all participants.

- www.nanoinitiative-bayern.de/index.php?id=697

FACULTY OF PHYSICS OPEN HOUSE

On May 4, the Faculty of Physics held an open house for the first time. Researchers and students showed to the public what physics has to offer in lectures, workshops and guided tours. Beside many CeNS research groups joining the event, the Center for NanoScience also presented its activities in the Lichthof of the LMU main building. The CeNS booth was supported by junior scientists from the Tinnefeld lab, fascinating visitors of all ages with their 3D nanoantenna models. In addition, the CeNS band “UnCeNSiert” added some musical delight to the open house.

CENS COMPANY VISITS

In 2019, CeNS organized two on-site company visits for its PhD students and postdocs. In March, a student group had the chance to visit Roche in Penzberg, a global pharma and diagnostics player located in the Munich area. The 15 participants were informed about early development in diagnostic research, met CeNS alumni Dr. Diana Pippig, Stefan Datz and Dr. Peter Röttgermann, and learned about career opportunities for physicists and chemists. The second visit went to the Infineon Campeon in Neubiberg in November. The CeNS student group learned about careers at Infineon, visited a test lab, and got detailed insight in one of Infineon's projects on electric drivetrains.

CENS RETREAT KLEINWALSERTAL

In March 2019, about 25 PhD students and postdocs set off for the CeNS retreat in the Söllerhaus in beautiful Kleinwalsertal. The intimate setting in the seminar house provided a perfect frame for getting to know each other and each other’s research better. After a scientific speed-dating, the participants presented their research in talks and during the poster session, followed by lively discussions. A workshop on Responsible Research made the attendees reflect on the scientific standards and implicit rules of their research community.

The program was complemented by two inspiring career talks, the academic track being presented by Prof. Bettina Lotsch, and the entrepreneurial track by Dr. Heinrich Grabmayr and Dr. Johannes Wöhrstein who are the faces behind the start-up DEOXY. Last but not least, the sunny weather and the snow offered wonderful opportunities for outdoor activities such as skiing or hiking.

CENS MEETS INDUSTRY

On July 19, CeNS meets Industry brought together members, graduate students and alumni, to foster the exchange between the academic world and the industrial sector. In five talks, different aspect from Venture Capital, consulting, to R&D in large and medium companies such as OHB Systems, Roche or Scanlab were covered.
In addition, CeNS and SFB1032 had organized a lunch for female junior scientists with the two female invited speakers of the event, Dr. Diana Pippig (Roche) and Dr. Ilina Kondofersky (OHB Systems). At the lunch, they exchanged career advice in a small group in an informal atmosphere. The talks were followed by the presentation of the two Nano Innovation Award 2019 winners and the summer party at the StuCafe Amalienstraße, as always with great music by the band "UnCeNSiert", food and drinks.

CENS B2RUN

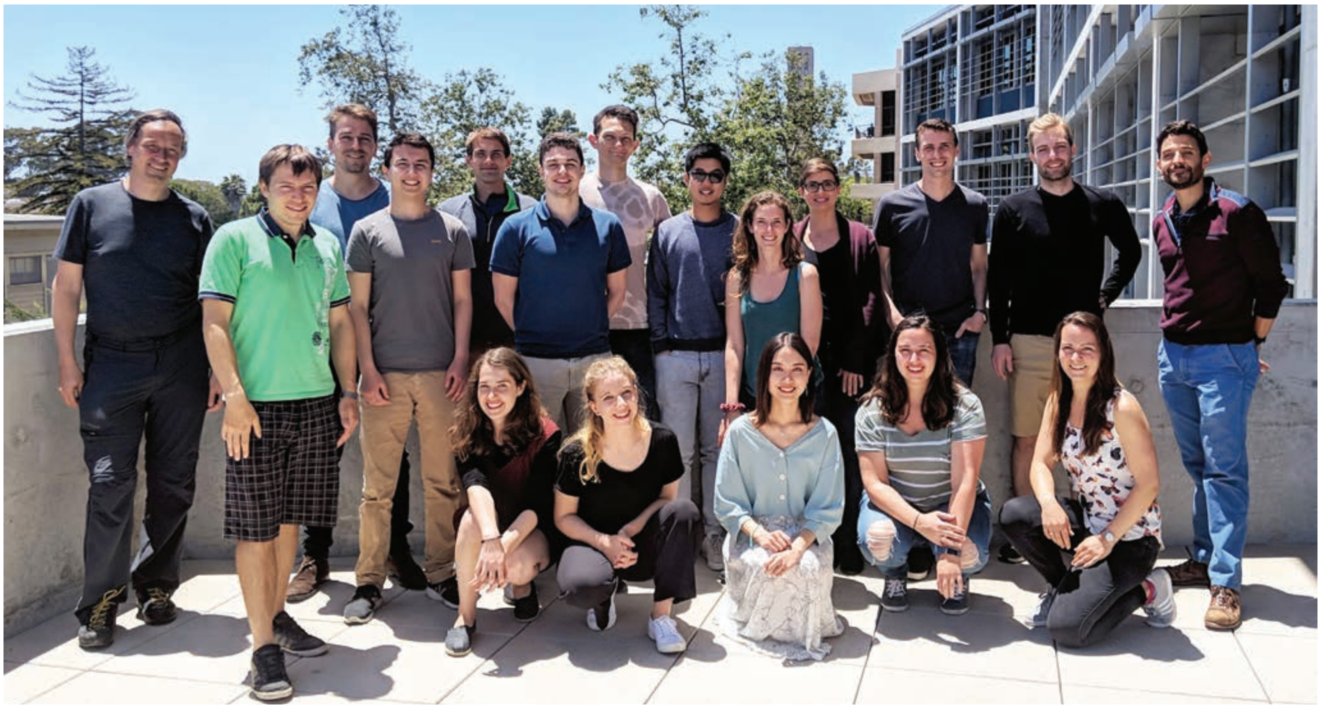
For the second time, a CeNS team entered the B2Run company competition in Munich. PhD students, postdocs, and administrative staff joined the "CeNSation" team and made it to the finishing line after running 6.1 km through the Olympic Park.

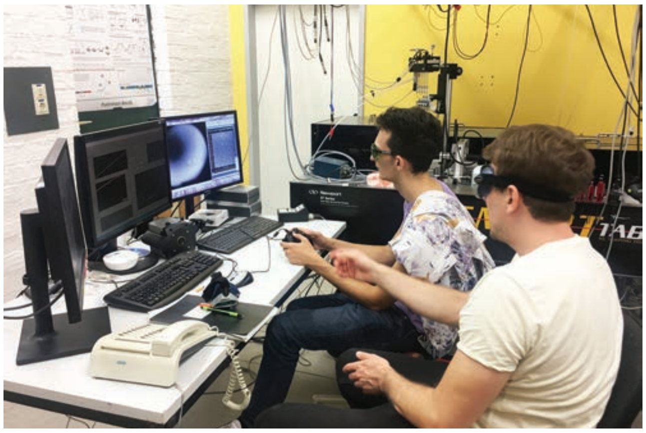
JUNIOR NANOTECH NETWORK

For the Junior Nanotech Network 2019 “Machine learning for molecular design and evolution” CeNS teamed up with the UC Santa Barbara for a joint PhD exchange program. The first part took place in Santa Barbara from May 30 to June 14. PhD students from LMU Munich, TU Munich, the University of Augsburg, and the MPI of Biochemistry enjoyed a challenging scientific program and the hospitality of their Californian hosts. One central part of the stay in Santa Barbara was dedicated to laboratory work. The visiting PhD students could choose between various modules that were organized and taught by the UCSB students, such as surface tension of DNA liquids, a machine learning approach to track single cells in complex 3D samples, high-throughput quantification of ribozyme activities, or single-molecule dynamic relaxation in disordered systems. The tutorials were focused on hands-on work so that the guest students could fabricate and measure their own samples, extend their technical skills and get to know laboratory routines. This way the students gained insight to a variety of methods that are applied in different areas of nanobioscience.

As a core element of the summer school, all participants attended a three-day workshop for Machine Learning. This workshop provided the basis for group projects dedicated to develop machine learning solutions for their own research tasks with support from the workshop instructors over the time course of the stay. The results were presented in a final meeting on the last day in Santa Barbara. Back in Munich, several participants started to incorporate their new knowledge on machine learning in their own PhD projects.

Besides sharing the common interest for science, the students connected very well on the personal level and spent their leisure time together engaging in activities such as a wine tasting trip to Santa Ynez valley, hiking in the beautiful Los Padres National Forest, a game night, and a beach barbecue.





During the second part of the JNN (September 9 – 27) the UCSB graduate students visited CeNS in Munich. After a Bavarian welcome breakfast on their first day, followed by a COMSOL workshop, the participants started with the lab rotations: small groups of two to three PhD students performed hands-on experiments in the labs on topics such as biomicrofluidics, single-molecule microscopy, thermogravitational trapping, DNA Origami, Bio-Nuclear Magnetic Resonance and much more at different CeNs groups. In addition, an excursion to the Physics department at the University of Augsburg and participation in a two-day retreat on Origin of Life research complemented the program.

The last week consisted of another highlight: All PhD students took part in the CeNS workshop "Evolving Nanosciences" at Venice International University. The PhD students presented their projects in two poster sessions. In addition, there was room for discussions with speakers and other participants in a charming Mediterranean atmosphere.

Besides the scientific program, the Californian participants also enjoyed a barbecue with CeNS PhD students and PIs, the vivid atmosphere of the Oktoberfest, a hiking trip in the Alps, and a farewell dinner in a Venetian restaurant.
Strong ties between German and Californian students were established not only by these educational and social activities but also by the unusual housing concepts, since private accommodation for all guests was provided by the host students. The 2019 JNN was a unique scientific as well as social experience for all participants and will certainly contribute to deepen existing collaborations and to establish new co-operations between CeNS Munich and UC Santa Barbara.

- www.cens.de/international/exchange-programs/jnn

SELECTED RESEARCH PROJECTS

1

RECONSTITUTION REVEALS HOW MYOSIN-VI SELF-ORGANISES TO GENERATE A DYNAMIC MECHANISM OF MEMBRANE SCULPTING

Benoit Rogez, Laeschkir Würthner, Anastasiia B. Petrova, Felix B. Zierhut, Dario Saczko-Brack, Maria-Ana Huergo, Christopher Batters, **Erwin Frey,** and **Claudia Veigel**

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It is well known that curvature-mediating proteins induce specific membrane shapes by direct interaction with the plasma membrane. It remains unclear, however, whether other cytoskeletal components constitute another route to remodel the membrane shape. Recently, a collaboration of the theoretical group led by Prof. Erwin Frey and the experimental group of Prof. Claudia Veigel discovered a novel route of generation, sensing and maintenance of membrane curvature through direct interactions of the motorprotein myosin-VI with the lipid membrane. The researchers showed, using reconstituted fluid supported lipid bilayers, super-resolution fluorescence microscopy and membrane-reshaping gold nanoparticles, that myosin-VI on its own remodels the membrane to form flower-shaped membrane pores. Furthermore, they showed that myosin-VI binding is highly curvature-dependent, resulting in recruitment of myosin-VI to saddle-shaped membrane geometries. The feedback between membrane geometry and myosin-VI binding leads to a morphological instability which establishes growing spatial patterns. The scientist developed a phenomenological model that describes the time-evolution of the protein-lipid interface as a nonlinear function of the local curvature. The model successfully reproduces qualitative and quantitative features of the system and explains this new route of protein-membrane interaction. The emerging route of protein-lipid interactions reshaping the membrane morphology opens up unexplored avenues of membrane remodeling and sets the foundation for future work on self-organisation of protein-lipid interfaces.

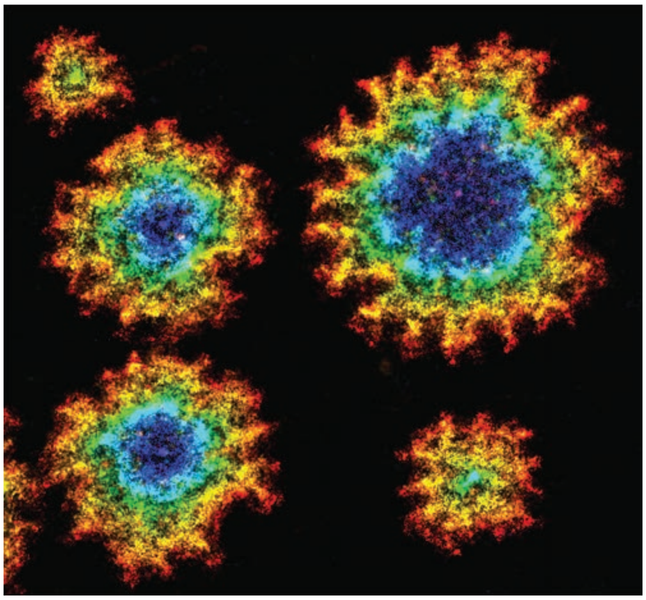

Fig. 1: Shown is the time evolution of the growing membrane pores (protein--lipid interface). An initially circular seed (blue) grows over time and generates a regular spatial structure (red), resulting in 'flower-shaped' membrane pores.

- **B. Rogez*, L. Würthner* A. B. Petrova, D. Saczko-Brack, M. Huergo, C. Batters, E. Frey, and C. Veigel:** *Reconstitution reveals how myosin VI self-organises to generate a dynamic mechanism of membrane sculpting;* Nature Communications 10, 3305 (2019).

2

VERTICAL, ELECTROLYTE-GATED ORGANIC TRANSISTORS SHOW CONTINUOUS OPERATION IN THE MA CM^{-2} REGIME AND ARTIFICIAL SYNAPTIC BEHAVIOUR

Jakob Lenz, Fabio del Giudice, FabianR. Geisenhof, Felix Winterer, and **R. Thomas Weitz**
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The "word-on-the-street" is, that organic transistors will never be able to support currents as high as inorganic materials such as silicon. This is best quantified in the current density, where highly integrated silicon transistors can support currents in the 10 MA/cm^2 regime, and organic transistors up to now at best 10 kA/cm^2.

We have now realized a novel electrolyte gated vertical organic field effect transistors (VOFETs), in which organic materials can show their full potential in terms of current density. One of the key steps is, that the device architecture allows the semiconductor deposition as last manufacturing step. In that way the semiconductor properties can be optimally maintained and remain uninfluenced by the successive process steps. We proved that even though the channels are only 40 nm short, the high gate coupling via the ionic liquid fully controls the charge carrier density in the channel without the observation of considerable short-channel effects. The electrolyte gated VOFETs sustain current densities above 3 MA cm^{-2} at -0.3 V bias, on/off current modulation of up to 10^8 and high transconductances of up to 5kS m^{-1}. The observed current densities are uniquely high for organic transistors. Furthermore, our VOFETs also perform well compared to SWCNT, MoS$_2$ and FIN-FETs. Our approach also provides an excellent platform for ultralow-power electronics as the transistor characteristics stay sufficiently intact down to an operation voltage of only 10 µV. This low-power operation is especially relevant for applications in artificial neural networks as memristive devices. We showed that depending on the operation voltage and exact transistor layout, the relative susceptibility of our VOFETs to short term and long term plasticity can be tuned. Additionally, switching event requiring energies as low as 10 fJ have been realised, which already outperforms CMOS neuromorphic devices and is only one magnitude larger than synaptic events used in the brain.

▪ **J. Lenz, F. del Giudice, F.R. Geisenhof, F. Winterer, R.T. Weitz:** *Vertical, electrolyte-gated organic transistors: continuous operation in the MA/cm^2 regime and use as low-power artificial synapses*; Nat. Nanotechnol. 14, 579–585 (2019).

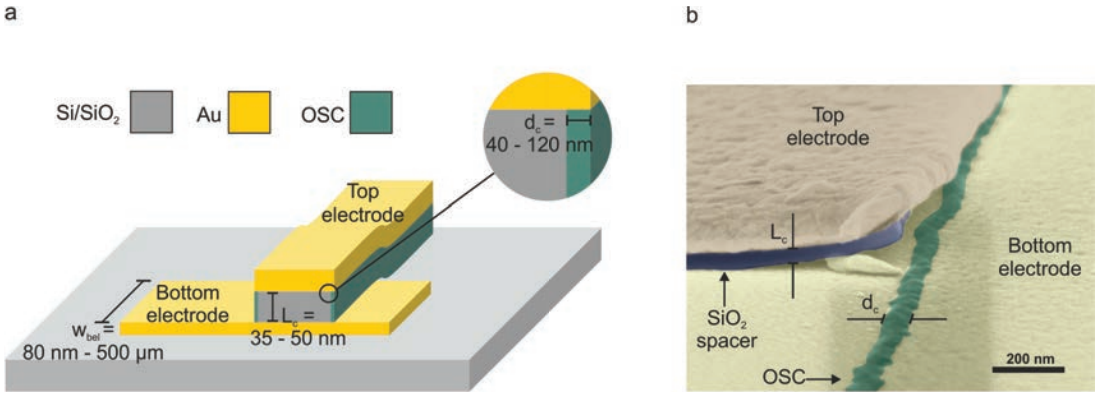

Fig. 1: (a) Scheme of the fully finished transistor and **(b)** coloured cross-sectional SEM image of a VOFET. The top electrode has bent upwards during the breaking of the device necessary to take the cross-sectional image.

3

STOCHASTIC NONLINEAR DYNAMICS OF CONFINED CELL MIGRATION

David B. Brückner, Nico Arlt, Alexandra Fink, Christoph Schreiber, **Joachim O. Rädler**, and **Chase P. Broedersz**

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Together with the Rädler lab we designed a minimal experimental system comprised of two adhesive squares connected by a thin bridge. On these patterns, single cells or pairs of cells repeatedly 'hop' back and forth between the square 'islands', and hundreds of cells of the same type moving in identical microenvironments could be monitored. The large amount of data produced by this approach can enable us to successfully apply tools from statistical physics to analyse cell motion and cell-cell interactions at a quantitative level.

To unravel the stochastic dynamics of confined cell migration on micropatterns, we adopted a data-driven modelling approach. The goal of this approach is to use experimentally determined statistical data to infer a stochastic equation of motion of a confined cell. This approach disentangles the dynamics into conceptually distinct components of cell motion: a deterministic component, which tells us what the cells do on average; and a stochastic one, which quantifies the inherent fluctuations in the cell dynamics.

With this framework, we established a new connection between the fields of cell migration and dynamical systems theory: the deterministic dynamics of a cell moving on the confining micropatterns can be analysed in terms of a geometrical representation of the trajectories in a two-dimensional plane of the cell’s position and velocity. This also enabled a classification of the behaviour of different cell types. Specifically, a breast cancer cell line (MDA-MB-231) was found to exhibit qualitatively different dynamics to a non-cancerous breast cell line (MCF10A): The cancerous cells perform deterministic oscillations described in terms of limit-cycles. By contrast, the non-cancerous cells are excitably bistable; they deterministically relax to either of two stable fixed points associated to each of the adhesive island. We have extendeded this work to patterns with different geometries and are now exploring cell-cell interactions on such confining patterns.

- **D. B. Brückner, A. Fink, J. O. Rädler, C. P. Broedersz:** *Disentangling the Behavioural Variability of Confined Cell Migration*; Journal of the Royal Society Interface 17, 20190689 (2020).

D. B. Brückner, A. Fink, C. Schreiber, P. Röttgermann, J. Rädler, C.P. Broedersz: *Stochastic nonlinear dynamics of confined cell migration in two-state systems;* Nature Physics 15, 595–601 (2019).

A. Fink, D. B. Brückner, C. Schreiber, P. Röttgermann, C. P. Broedersz, J. Rädler: *Area and geometry dependence of cell migration in asymmetric two-state micropatterns;* Biophysical Journal, 118, 552-564 (2019).

4

FROM OPTICAL TO CHEMICAL PLASMONIC HOT SPOTS

Julian Gargiulo, Yi Li, Rodrigo Berte, **Stefan A. Maier, Emiliano Cortés**
■ www.hybridplasmonics.org

We discuss a series of techniques to spatially map and image plasmonic nanoscale reactivity at the single photocatalyst level. We show how to optimize the reactivity of carriers by manipulating their excitation and decay mechanisms in plasmonic nanoparticles. In addition, the tailored generation of non-thermal phonons in metallic nanostructures and their dissipation is shown as a promise to understand and exploit thermal photocatalysis at the nanoscale. Understanding and controlling these processes is essential for the rational design of solar nanometric photocatalysts.

■ **J. Gargiulo, Y. Li, R. Berte, S. A. Maier, E. Cortés:** *From optical to chemical plasmonic hot spots;* Accounts of Chemical Research 52, 2525-2535 (2019), Cover Article.

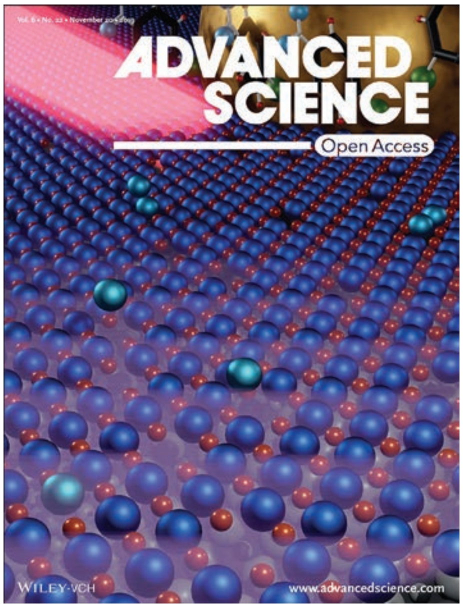
5

DYNAMICS OF PHOTO-INDUCED SURFACE OXYGEN VACANCIES IN METAL-OXIDE SEMICONDUCTORS STUDIED UNDER AMBIENT CONDITIONS

Daniel Glass, **Emiliano Cortés**, Sultan Ben-Jaber, Thomas Brick, William J Peveler, Christopher S Blackman, C. R Howle, Raul Quesada-Cabrera, Ivan P Parkin, and **Stefan A. Maier**
■ www.hybridplasmonics.org

Surface-enhanced Raman spectroscopy (SERS) is a powerful analytical technique commonly used in the detection of traces of organic molecules. The mechanism of SERS is of a dual nature, with Raman scattering enhancements due to a combination of electromagnetic (EM) and chemical contributions. In conventional SERS, the EM component is largely responsible for the enhancement, with the chemical contribution playing a less significant role. An alternative technique, called photo-induced enhanced Raman spectroscopy (PIERS) has been recently developed, using a photo-activated semiconductor substrate to give additional chemical enhancement of Raman bands over traditional SERS. This enhancement is assigned to surface oxygen vacancies (V_o) formed upon pre-irradiation of the substrate. In this work, the exceptional chemical contribution in PIERS allows for the evaluation of atomic V_o dynamics in metal oxide surfaces. This technique is applied to study the formation and healing rates of surface-active V_o in archetypical metal-oxide semiconductors, namely, TiO_2, WO_3, and ZnO. Contrary to conventional analytical tools, PIERS provides intuitive and valuable information about surface stability of atomic defects at ambient pressure and under operando conditions, which has important implications in a wide range of applications including catalysis and energy storage materials.

- **D. Glass, E. Cortés, S. Ben-Jaber, T. Brick, W. J Peveler, C. S Blackman, C. R Howle, R. Quesada-Cabrera, I. P Parkin, S. A. Maier:** *Dynamics of Photo-Induced Surface Oxygen Vacancies in Metal-Oxide Semiconductors Studied Under Ambient Conditions;* Advanced Science 6 (22), 1901841 (2019).



6

LOCALIZATION-BASED FLUORESCENCE CORRELATION SPECTROSCOPY TO QUANTIFY ABSOLUTE NUMBERS AND TURNOVER TIMES SCALES OF SURFACE BINDING EVENTS

Johannes Stein, Florian Stehr, Patrick Schueler, Philipp Blumhardt, Florian Schueder, Jonas Mücksch, **Ralf Jungmann,** and **Petra Schwille**

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- www.biochem.mpg.de/jungmann

Single-molecule localization microscopy (SMLM) has revolutionized optical microscopy, extending resolution down to the level of individual molecules. In combination with surface integrated Fluorescence Correlation Spectroscopy, it can also be employed to quantify the turnover time scales of surface binding events, e.g. for receptor-ligand or generally protein-membrane interactions. However, the precise counting of surface bound molecules relies on preliminary knowledge of the blinking behavior of individual targets or on a calibration to a reference. In close collaboration with the Jungmann group, we developed localization-based fluorescence correlation spectroscopy (lbFCS) as the first absolute molecular counting approach for any analyses based on PAINT microscopy and SMLM in general. We demonstrated that lbFCS overcomes the limitation of previous DNA-PAINT counting and allows the quantification of target molecules independent of the localization cluster density.

- **Stein, J.*, Stehr, F.*, Schueler, P., Blumhardt, P., Schueder, F., Mücksch, J., Jungmann, R., Schwille, P.:** *Towards absolute molecular numbers in DNA-PAINT;* Nano Lett 19, 8182-8190 , DOI: 10.1021/acs.nanolett.9b03546 (2019).

7

FISSION OF LIPID-VESICLES BY MEMBRANE PHASE TRANSITIONS IN THERMAL CONVECTION

Patrick W. Kudella, Katharina Preißinger, Matthias Morasch, Christina F. Dirscherl, **Dieter Braun, Achim Wixforth,** and **Christoph Westerhausen**

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- www.physik.uni-augsburg.de/exp1/mitarbeiter/02_seniors/westerhausen_christoph/
- www.physik.uni-augsburg.de/exp1/mitarbeiter/01_profs/wixforth_achim/

We here show an easy and reliable way to divide lipid vesicles. While vesicles are widely regarded as suitable protocells, the division of such protocells remains largely unexplored. Because of the lack of internal, cell-like fission mechanisms, the leading cause for vesicle division must be the environmental settings and membrane properties only.

The mechanism described here shows a division pathway that combines a steep temperature-gradient and a parabolic flow profile, the combination of which reliably divides lipid vesicles. Without the need for additional, chemically induced processes, vesicles with a first order membrane phase transition are prone to fission by this mechanism.

In a thermal convection chamber we find a significant reduction of the size distribution for a wide range of vesicle sizes cycling through cold and hot regions and thus undergoing membrane phase transitions repeatedly. Tracing single vesicles in a capillary with a steep temperature gradient we monitored vesicle shape transformations resulting in fission. From these observations we deduce the underlying mechanism. Domaining due to the experienced shear forces causes a separation of vesicle volume by tether-like surface domains which eventually rupture during the phase transition back to the gel-like phase.

Both capillary and convection chamber are experimental realizations of hydrothermal microenvironments. They combine non-uniform flow profiles with rapid temperature-changes, a setting which is plausible in the context of the Origin of Life and is known to have the ability to accumulate dissolved molecules from strongly diluted solutions and provide a mechanism for the formation of lipid-vesicles.

These results for the first time show the potential of phase transitions of lipid membranes for the

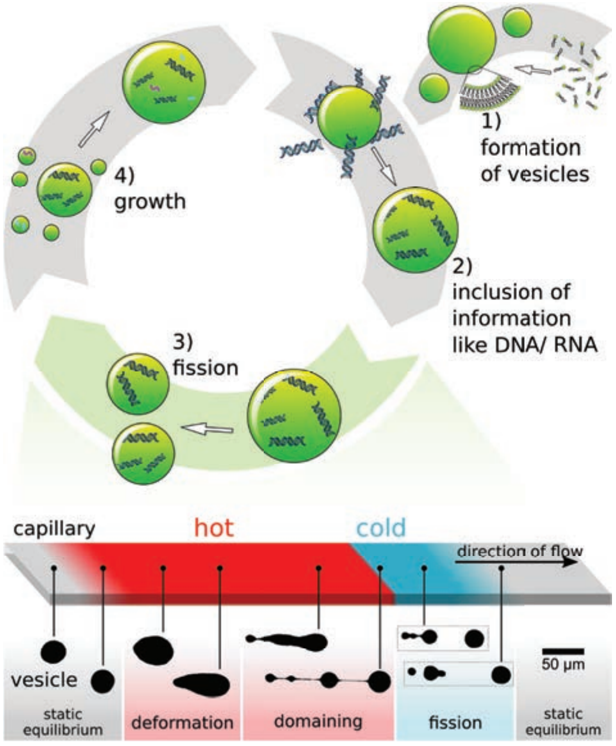

Fig. 1: Over time, more and more vesicles that contain various molecules may have formed in a cycle of growth and division. They possibly made countless random experiments possible that ultimately led to a chemical evolution and then to the formation of the first living cells. For the division, the vesicles must flow through a temperature gradient. In the first step, the vesicle surface greatly increases, which leads to deformation and division (lower figure, red area) as a new equilibrium state. In the second step, the front section contracts due to the abrupt cooling, which is hardly possible due to the, almost, spherical shape. The tension of the lipid membrane ultimately results in division.

crucial development of a protocell cycle during the origin of life. Vesicles could be a step on the way to protocells that enclose, replicate, transport, shield, and distribute information, e.g. in the form of nucleic acids, without the sophisticated division mechanisms of evolved modern cells. Prebiotically plausible protocells probably had much less sharp phase transitions. However, the same physics as for our protocell model with a structurally simple membrane would apply.

- **P. W. Kudella, K. Preißinger, M. Morasch, C. F. Dirscherl, D. Braun, A. Wixforth and C. Westerhausen:** *Fission of Lipid-Vesicles by Membrane Phase Transitions in Thermal Convectio;* Sci. Rep., Dez. 2019, 9, 18808.

8

MODULAR DESIGN OF PATTERN FORMING PROTEIN SYSTEMS

Philipp Glock, Fridtjof Brauns, Jakob Halatek, **Erwin Frey,** and **Petra Schwille**

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Because of its compositional simplicity of only two proteins and a membrane, the MinDE system from *Escherichia coli* has in the past years been invaluable for deciphering the mechanisms of spatiotemporal self-organization in cells. In a fruitful combination of experiment and theory, we explored the potential of reducing the complexity of this system even further, by identifying key functional motifs in the effector MinE that could be used to design pattern formation from scratch. We could show that starting from a minimal MinE-MinD interaction motif, pattern formation can be obtained by adding either dimerization or membrane-binding motifs, and that the pathways underlying pattern formation are recruitment-driven cytosolic cycling of MinE and recombination of membrane-bound MinE.

- **Glock, P., Brauns, F., Halatek, J., Frey, E., Schwille, P.:** *Design of biochemical pattern forming systems from minimal motifs;* eLife 8:e48646, DOI: 10.7554/eLife.48646 (2019).

9

HEATED GAS BUBBLES ENRICH, CRYSTALLIZE, DRY, PHOSPHORYLATE, MELT AND ENCAPSULATE PREBIOTIC MOLECULES

Matthias Morasch, Jonathan Liu, Christina F. Dirscherl, Alan Ianeselli, Alexandra Kühnlein, Kristian Le Vay, Philipp Schwintek, Saidul Islam, Mérina K. Corpinot, Bettina Scheu, Donald B. Dingwell, **Petra Schwille, Hannes Mutschler,** Matthew W. Powner, **Christof B. Mast**, and **D. Braun**

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The possibilities of non-equilibrium settings was greatly expanded by the Braun group in collaboration with the Powner and Mutschler group by exploring water-gas interfaces in a temperature gradient (Nature Chemistry 2019, doi.org/10.1038/s41557-019-0299-5). The continuous flow of evaporation at a 20-30K warmer gas-water interface provided accumulation of RNA and salts for enhanced RNA catalysis, triggered gelation of self-complementary 36mers, gave rise to encapsulation with lipids where the inside RNA concentrations were 20-fold enhanced. The accumulation also lead to crystallization at bubbles of the RNA progenitor molecule RAO. As the interface moved periodically by the condensation and dripping of pure water bubbles on the cold gas side of the interface, fast wet dry cycles are implemented at the warm accumulating side of the gas-water interface. This was shown to provide enhanced ways for condensation reactions at low temperatures, shown experimentally by the phosphorylation of nucleosides. Moreover, the salt cycling in these settings by the falling droplets into provided a way to separate strands (Angewandte Chemie 2019, doi:10.1002/anie.201907909). This is another way how non-equilibrium settings allow to oscillate salt concentrations on a fast scale in an evaporation-protected pore space. With these novel findings, strand separation at low salt can be combined with fast wet-dry cycles under conditions of co-accumulating nucleotides and salts for activation and replication. The Braun group at this time develops portable machines optimized for fume hoods of collaborating chemical labs, enabling the distribution of above non-equilibrium settings.

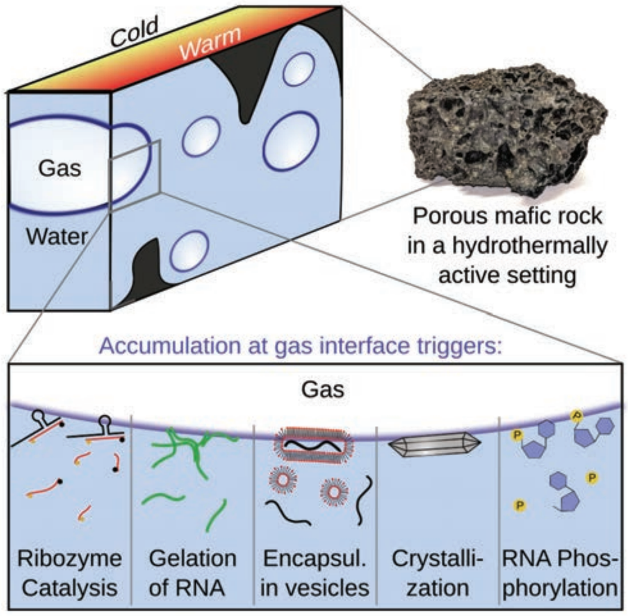

Fig. 1: DNA accumulation at gas bubbles in a thermal gradient. Volcanic rocks in shallow hydrothermal settings are subjected to water cycles in their pore spaces, which are of both primary (magmatic vesicles) and secondary (fractures) origin. The heat causes vaporization at the warm side. At the gas interface, molecules are accumulated by the continuous capillary flow on the warmer side of the gas–water interface. As shown experimentally, this environment can enhance the catalytic activity of ribozymes, trigger the formation of a hydrogel from self-complementary RNA, encapsulate and melt oligonucleotides such as aptamers in vesicle aggregates, trigger their subsequent fission, drive the crystallization of the precursor ribose aminooxazoline (RAO) and initiate the phosphorylation of RNA nucleosides. drive the crystallization of the precursor ribose aminooxazoline (RAO) and initiate the phosphorylation of RNA nucleosides.

- **M. Morasch, J. Liu, C.F. Dirscherl, A. Ianeselli, A. Kühnlein, K. Le Vay, P. Schwintek, S. Islam, M.K. Corpinot, B. Scheu, D.B. Dingwell, P. Schwille, H. Mutschler, M.W. Powner, C.B. Mast & D. Braun**: *Heated gas bubbles enrich, crystallize, dry, phosphorylate and encapsulate prebiotic molecules;* Nature Chemistry, doi.org/10.1038/s41557-019-0299-5 (2019).

Alan Ianeselli, Christof B. Mast and Dieter Braun: *Periodic Melting of Oligonucleotides by Oscillating Salt Concentrations triggered by Microscale Water Cycles inside Heated Rock Pores*; Angewandte Chemie, doi.org/10.1002/ange.201907909 (2019).

10

CAVITY-CONTROL OF INTERLAYER EXCITONS IN VAN DER WAALS HETEROSTRUCTURES

Michael Förg, Leo Colombier, Robin K. Patel, Jessica Lindlau, Aditya D. Mohite, Hisato Yamaguchi, M. Mikhail Glazov, David Hunger, and **Alexander Högele**

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The work reports the results of a collaborative experimental and theoretical study of light-matter coupling between an optical micro-cavity and a semiconductor van der Waals heterostructure. Using $MoSe_2$-WSe_2 heterobilayer as a representative material for the class of vertically stacked heterostructures built from novel two-dimensional materials, we performed a detailed analysis of optical absorption and emission spectra at cryogenic temperatures. As a key result of our work, we determined quantitatively the strength of light-matter coupling for $MoSe_2$-WSe_2 interlayer excitons embedded in a fiber-based optical micro-cavity, and demonstrated Purcell enhancement of interlayer exciton photoluminescence in the weak coupling regime.

- **M. Förg, L. Colombier, R. K. Patel, J. Lindlau, A. D. Mohite, H. Yamaguchi, M. M. Glazov, D. Hunger, A. Högele:** *Cavity-control of interlayer excitons in van der Waals heterostructures*; Nat. Commun. 10, 3697 (2019).

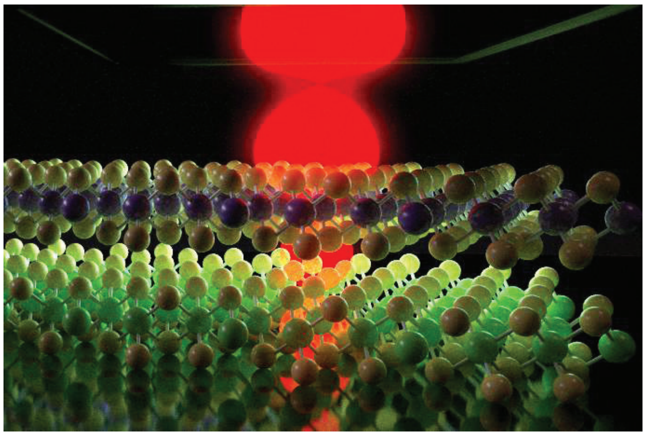

Fig. 1: Artistic view of light-matter coupling between a semiconductor heterostack and a fiber micro-cavity. Image by C. Hohmann.

11

THE FREE ENERGY LANDSCAPE OF RETROVIRAL INTEGRATION

Willem Vanderlinden, Tine Brouns, Philipp U. Walker, Pauline Kolbeck, Lukas Milles, Wolfgang Ott, Philipp Nickels, Zeger Debyser, and **Jan Lipfert**
■ **www.molecularbiophysics.physik.lmu.de**

Integration is the covalent insertion of a viral genome into the host DNA and a critical step in the retroviral replication cycle: It is a requirement for the virus to replicate and it essentially irreversible for the host. The integration reaction is catalyzed by the viral enzyme integrase that assembles as a multimer on viral DNA ends to form the intasome DNA-protein complex. Because intasomes are loaded with a single viral DNA, there is no catalytic turnover, which makes it critical to establish strand transfer in a highly efficient manner. Yet, the chemistry is iso-energetic, and would intrinsically yield no more than 50% strand transfer product. It is an open question whether and how retroviruses have evolved to overcome this fundamental limitation.

Here, we have used intasomes of prototype foamy virus (PFV) to study the integration reaction in vitro, using a combination of bulk, AFM imaging and single-molecule magnetic tweezers assays. We find that the reaction has a ~90% yield and is driven by the energy stored in the mechanical strain of the target DNA. In addition, we find that the intasome complex has multiple auxiliary binding interfaces in addition to the active site. The auxiliary binding interfaces help position the target DNA in the active, facilitate an efficient target search, and create an overall downhill free energy landscape. The resulting final strand transfer complex is extremely stable and long-lived, with an extrapolated lifetime at zero forces of ~6 months, which suggests that need for a resolving factor *in vivo*.

Our work provides a comprehensive, mechanistic picture of retroviral integration, with exciting biological implications. In addition, the experimental platform that we have developed is already being used to probe retroviral integration in more complex contexts and for different viruses.

■ **W. Vanderlinden, T. Brouns, P. U. Walker, P. Kolbeck, L. Milles, W. Ott, P. Nickels, Z. Debyser, and J. Lipfert:** *The Free Energy Landscape of Retroviral Integration*; Nature Comm. 10:4738

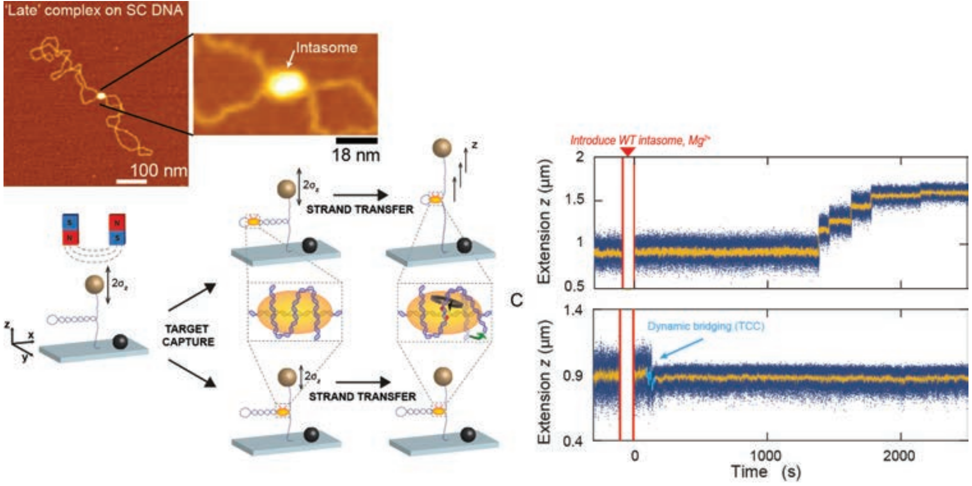

Fig. 1: Top: AFM image of an intasome complex complex on target DNA after reaction. The intasome complex remains bound and holds the DNA ends together. Bottom: Magnetic tweezers assay to probe the integration reaction on supercoiled DNA. We observe two signatures after adding intasomes to supercoiled DNA held in magnetic tweezers: a reduction in fluctuations (bottom trace) due to binding and DNA bridging of intasomes and step-wise increases in DNA extension due to removal of supercoils after reaction.

12

TEMPERATURE DEPENDENCE OF AMBIPOLAR CHARGE CARRIER DIFFUSION IN HYBRID HALIDE PEROVSKITE THIN FILMS

Alexander Biewald, Nadja Giesbrecht, Pablo Docampo, Richard Ciesielski, **Achim Hartschuh**, and **Thomas Bein**

- https://physchem.cup.uni-muenchen.de/hartschuh
- http://bein.cup.uni-muenchen.de

Perovskite-based thin-film solar cells today reach power conversion efficiencies of more than 22%. Methylammonium lead iodide (MAPI) is prototypical for this material class of hybrid halide perovskite semiconductors and at the focal point of interest for a growing community in research and engineering. Here, a detailed understanding of the charge carrier transport and its limitations by underlying scattering mechanisms is of great interest to the material's optimization and development. We performed an all-optical study of the charge carrier diffusion properties in large-crystal MAPI thin films in the tetragonal crystal phase from 170 K to room temperature. We first probed the local material properties of individual crystal grains within a MAPI thin film and identified a thermally activated decay channel with an activation energy of 200 meV that is probably caused by surface defects. We then found a steady decrease of the charge carrier diffusion constant within single grains with increasing temperature. From the resulting charge carrier mobility, we derived a power law dependence of $\mu \alpha T^m$ with $m = -(1.8 \pm 0.1)$. We further studied the temperature-dependent mobility of the orthorhombic crystal phase from 50 to 140 K and determined a distinctly different exponent of $m = -(1.2 \pm 0.1)$. The observed scaling behavior supports the theoretical model of lattice fluctuations and optical phonons as the dominant scattering mechanisms for charge carriers in large-crystal MAPI thin films in the tetragonal phase. The presented findings contribute to our understanding of charge carrier transport in hybrid halide perovskite semiconductors and its limitations.

- **A. Biewald, N. Giesbrecht, T. Bein, P. Docampo, A. Hartschuh, R. Ciesielski:** *Temperature dependent ambipolar charge carrier mobility in large crystal hybrid halide perovskite thin films*; ACS Appl. Mater. Interfaces 11, 20838 (2019).

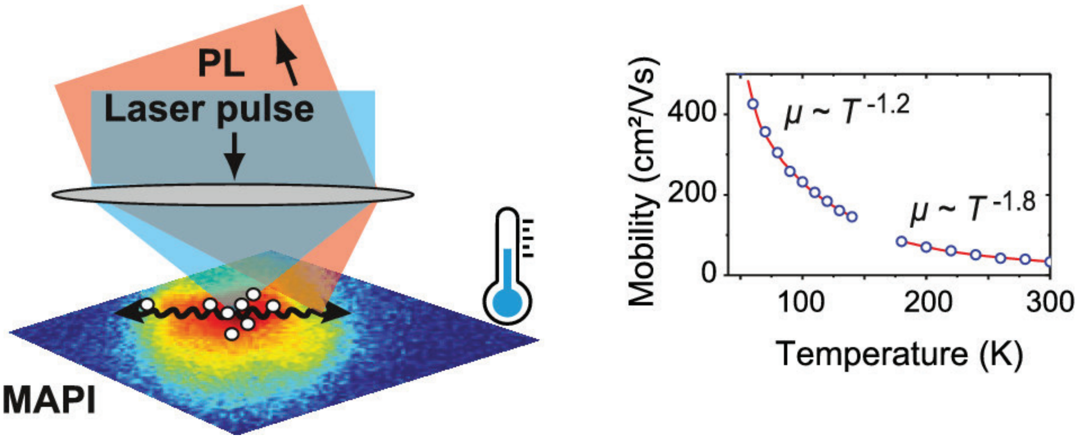

Fig. 1: Experimental approach and obtained temperature dependent ambipolar charge carrier mobility in large crystal hybrid halide perovskite thin films.

13

QUANTITATIVE SINGLE-MOLECULE THREE-COLOR FÖRSTER RESONANCE ENERGY TRANSFER BY PHOTON DISTRIBUTION ANALYSIS

Anders Barth, Lena Voith von Voithenberg, and **Don C. Lamb**
- www.cup.lmu.de/pc/lamb

In single-pair Förster Resonance Energy Transfer (FRET), energy is transferred non-radiatively from a donor molecule to an acceptor molecule. By monitoring the fluorescence intensity and/or lifetime, it is possible to measure distances on the molecular scale and thereby determine the conformation and dynamics of biomolecules one the single molecule level. By adding a third color, it is possible to follow three distances simultaneously. In theory, this is straightforward but in practice it is very challenging. There are many correction factors that need to be taken into account and the statistics are low making the distribution of measured FRET efficiencies broad. To overcome many of the challenges presented by three-color FRET, Anders Barth developed a Maximum Likelihood approach to calculate the photon-distribution in three color experiments. All of the necessary corrections to convert the measured fluorescence into three distances are performed in the analysis. The analysis approach was verified on simulated data and on double-stranded DNA before being applied to the heat shock protein 70 BiP. By being able to track three distances simultaneously on the same protein, it is no possible to investigate coordinated motions in proteins. This opens new possibilities for understanding how proteins work where allosteric effects are common for controlling function.

- **A. Barth, L. Voith von Voithenberg, and D.C. Lamb:** *Quantitative Single-Molecule Three-Color Förster Resonance Energy Transfer by Photon Distribution Analysis*; J Phys Chem B. 123: 6901–6916 (2019).

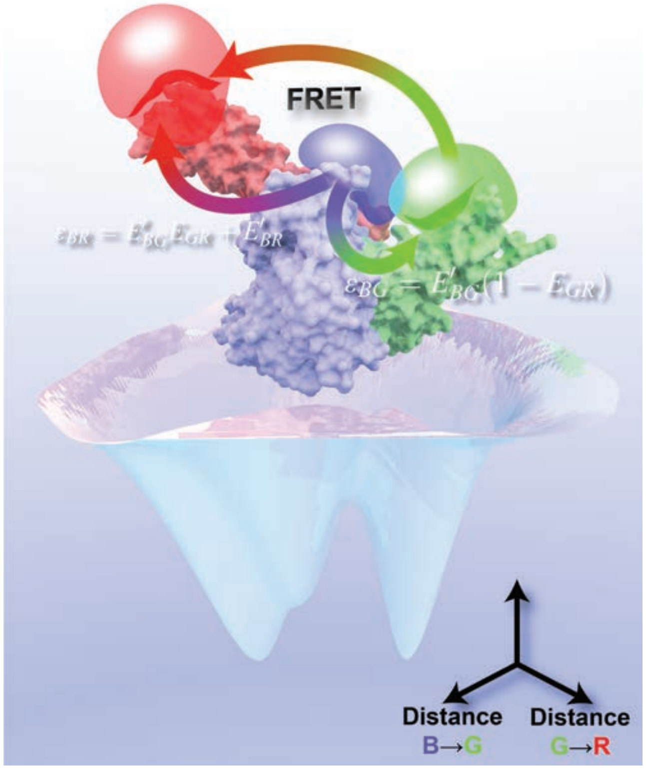

Fig. 1: The structure of the Hsp70 protein BiP in the open conformation is shown with three fluorophores attached. Below is the conformational energy landscape of the protein, that can be extracted from the determination of the FRET efficiency between the three fluorophores (given by the formulas).

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VIDEO-RATE SCANNING TUNNELING MICROSCOPY OF SURFACE DIFFUSION

Ann-Kathrin Henß, Sung Sakong, Philipp K. Messer, Joachim Wiechers, Rolf Schuster, **Don C. Lamb,** Axel Groß, and **Joost Wintterlin**

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Surface diffusion of adsorbed particles is an important process in heterogeneous catalysis. It is responsible for the mixing of the adsorption layer and also for the rate at which the particles can reach active sites, the sites at which a critical chemical step takes place. By means of a home-built variable-temperature scanning tunneling microscope (STM) that can operate at video-rates atomically resolved movies of diffusing particles have been recorded. Experiments were performed with a ruthenium surface that was completely covered by a layer of CO molecules plus a low concentration of oxygen atoms that were embedded in the CO layer. The system modelled an industrial situation in which, because of the high gas pressure, the surface of the employed catalyst is usually covered by a dense layer of adsorbed particles. An open question has been how the particles can move on such a crowded surface.
In the STM movies the O atoms were seen to travel through the layer of CO molecules. Using a particle detection and tracking algorithm that had been developed for flourescence-labelled molecules in biological systems, trajectories of the O atoms could be extracted from the data. The analysis showed that the O atoms move through the CO layer almost as fast as on the empty ruthenium surface. To understand this unexpected observation the energy profiles of all surface processes that might play a role were calculated by DFT. It turned out that at a temperature where the O atoms are mobile there are also frequent density fluctuations in the layer of CO molecules. As long as an O atom is completely surrounded by CO molecules it is trapped like in a cage, but because of the high rates of CO fluctuations these also affect the CO molecules near the O atom. When this happens, the CO cage opens and the O atom can jump to a neighboring site. This "door-opening" represents a new type of diffusion mechanism in 2D lattices, and it can explain a high mobility on a densely covered surface. Such effects may generally operate in catalytic reactions.

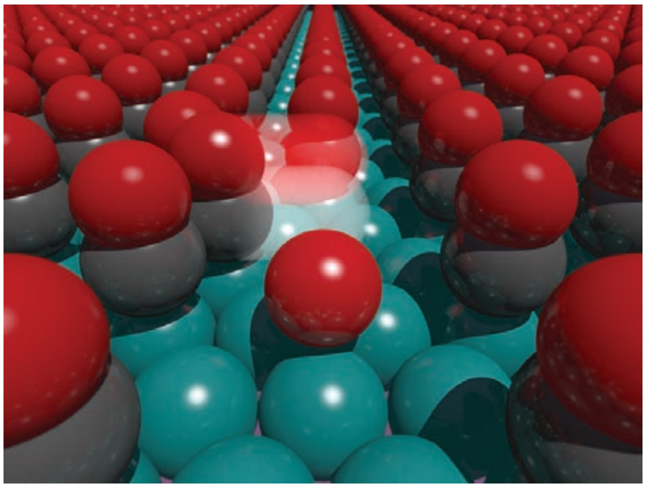

Fig. 1: Model of an adsorbed oxygen atom on a Ru(0001) surface. The O atom is embedded in a dense layer of CO molecules but can diffuse across the surface when neighboring CO molecules change sites.

- **A.-K. Henß, S. Sakong, P. K. Messer, J. Wiechers, R. Schuster, D. C. Lamb, A. Groß, J. Wintterlin:** *Density fluctuations as door-opener for diffusion on crowded surfaces;* Science, 10.1126/science.aav4143 (2019).

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LIGHT CAGES

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The *Light Cage* is a collaborative project between the Chair in Hybrid Nanosystems of LMU in Munich and The Fiber Sensor Group at the Institute of Photonic Technology in Jena. The *Light Cage* is a new concept in optical waveguides. A 3D nano-printer was used to fabricate polymer bars that can trap and guide light in a hollow core. The developed waveguides exhibit extraordinary properties such as (1) diffractionless propagation in "quasi-air" over more than a centimeter distance within the ultraviolet, visible and near-infrared spectral domains, (2) unique side-wise direct access to the hollow core via open spaces between the strands speeding up gas diffusion times by at least a factor of 10^4, and (3) an extraordinary high fraction of modal fields in the hollow section (>99.9%). With these properties, the light cage can overcome the limitations of current planar hollow core waveguide technology, allowing unprecedented future on-chip applications within quantum technology, ultrafast spectroscopy, bioanalytics, acousto-optics, optofluidics, and nonlinear optics.

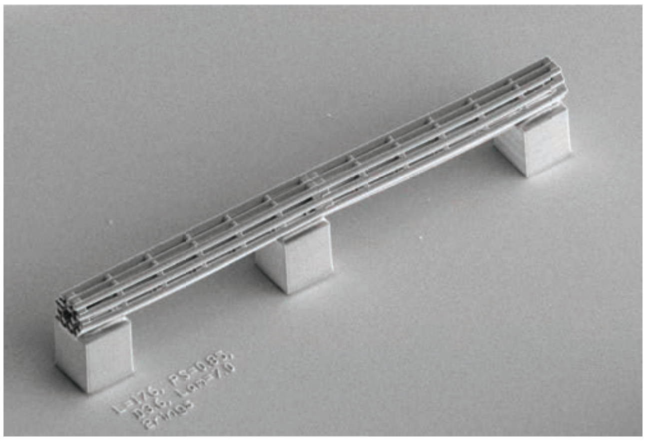

Fig. 1: This image shows the concept of an on-chip novel waveguide. A 3D nano-printer was used in the Chair in Hybrid Nanosystems to fabricate polymer bars that can trap and guide light in a hollow core. The resulting photonic structure can be used for several applications such as bio-sensing, gas spectroscopy or quantum information processing. This image was selected for the CeNS Kalender 2020.

■ **B. Jang, J. Gargiulo, R. F. Ando, A. Lauri, S. Maier, and M. Schmidt:** *Light Guidance in Photonic Band Gap Guiding Dual Ring Light Cages Implemented by Direct Laser Writing;* Optics Letters , https://doi.org/10.1364/OL.44.004016 (2019).

B. Jang, J. Gargiulo, M. Ziegler, R. F. Ando, U. Hübner, S. A. Maier, and M. A. Schmidt: *Fine-tuning of the optical properties of hollow-core light cages using dielectric nanofilms;* https://doi.org/10.1364/OL.45.000196. (2020).

16

A CONSERVED ATP- AND SCC2/4-DEPENDENT ACTIVITY FOR COHESIN IN TETHERING DNA MOLECULES

Pilar Gutierrez-Escribano, Matthew Newton, Aida Llauró, Jonas Huber, Loredana Tanasie, Joseph Davy, Isabel Aly, Ricardo Aramayo, Alex Montoya, Holger Kramer, **Johannes Stigler,** David Rueda, and Luis Aragon
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Interphase chromosomes in higher eukaryotes are hierarchically structured on different levels, ranging from DNA wrapped around histones, to chromatin fibers, up to large chromosomal domains encompassing hundreds of kilobases. Hi-C experiments have shown that these topologically associating domains (TADs), which consist of regions of increased interactions of certain genomic regions, are a structural feature of all higher eukaryotes. TADs are generally isolated by domain boundaries from adjacent regions.

Sister chromatid cohesion and the establishment of topologically associating domains (TADs) in interphase chromosomes requires the SMC complex cohesin to act as a linker protein between chromatids. How cohesin tethers chromatids remains poorly understood.

We have used DNA curtains to visualize single cohesin complexes as they interact with DNA molecules and establish tethering between adjacent strands of DNA. We show in optical tweezers assays that cohesin complexes create DNA loops in cis and tether DNAs in trans in the presence of Scc2/Scc4 and ATP, demonstrating a conserved activity from yeast to humans. Cohesin forms two classes of tethers: "permanent bridges" resisting forces over 65 pN and force-sensitive "reversible bridges" that dissolve at about 10 pN, indicating that there are multiple modes of interaction.

We finally demonstrate that in the presence of Scc2/Scc4 and ATP, cohesin can compact linear DNA molecules stretched by very low force (below 1 pN), consistent with the possibility that, like condensin, cohesin is also capable of loop extrusion.

▪ **P. Gutierrez-Escribano *et al.*:** *A conserved ATP- and Scc2/4-dependent activity for cohesin in tethering DNA molecules;* Science Advances 10.1126/sciadv.aay6804 (2019).

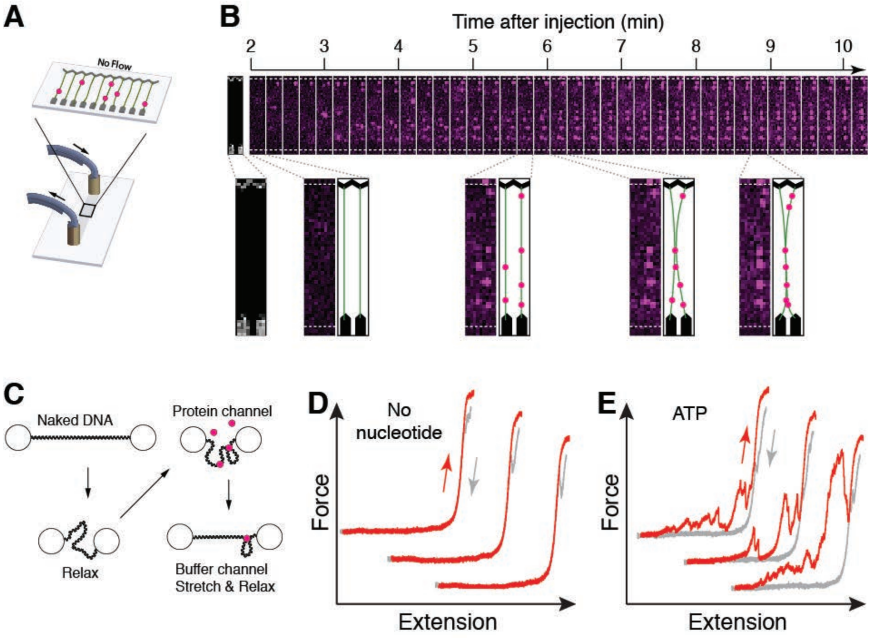

Fig. 1: Cohesin-Scc2/Scc4 and ATP tether DNA molecules. (A) DNA curtains assay to visualize fluorescently tagged cohesin complexes on DNA. (B) Cohesin complexes tether adjacent strands of DNA. (C) Optical tweezers workflow to test cohesin-mediated cis-loop formation. (D),(E) Cohesin-Scc2/4 does not form loops in the absence of nucleotide but does so in the presence of ATP.

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NANORESOLUTION REAL-TIME 3D ORBITAL TRACKING FOR STUDYING MITOCHONDRIAL TRAFFICKING IN VERTEBRATE AXONS IN VIVO

Fabian Wehnekamp, Gabriela Plucinska, Rachel Thong, Thomas Misgeld, and **Don C. Lamb**
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One of the ultimate experiments in biophysics is to be able to following individual molecules and particles as they perform their function in living organisms. Until now, this has only been the subject of science fiction as the adequate methods with such capabilities are still missing. Here, we present single particle tracking technique that is capable of following individual objects in living zebra fish embryos. The method is based upon the 3D orbital tracking method developed in the group of Professor Lamb. The laser is orbited about an object and the resulting signal used to follow the object in real-time with nanometer precession. Several upgrades were made to the system to allow the method to be able to follow individual particles over distances larger than 100 µm. Here, Fabian Wehnekamp from the group of Professor Lamb made several upgraded to the system and then used the method to follow mitochondria labelled with photoactivatable green fluorescence proteins in living zebra fish embryos. Hereby, he discovered a new transport behavoir and dissected the interplay between the different states.

■ **F. Wehnekamp, G. Plucinska, R. Thong, T. Misgeld, and D.C. Lamb:** Nanoresolution real-time 3D orbital tracking for studying mitochondrial trafficking in vertebrate axons in vivo; eLife Sciences. 8: 655 (2019).

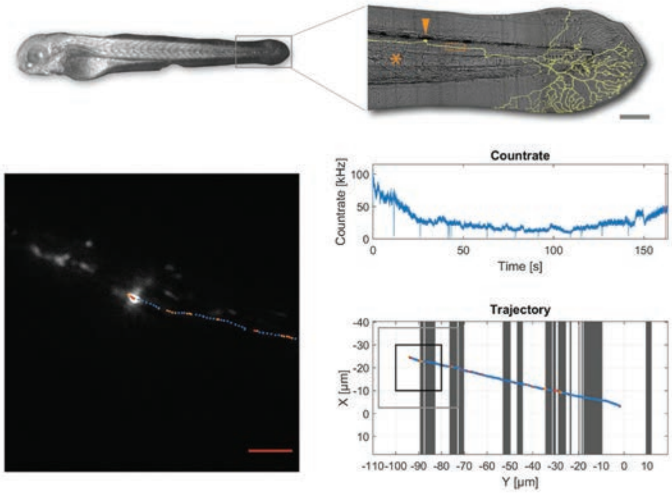

Fig. 1: Upper panel: A wide field image of a Zebra fish embryo is shown with a zoom in on the fin region where the Rohon-Beard neuron is highlighted. Lower panel: A wide-field image of a region of the neuronal axon is shown along with the trajectory of a single mitochondria being tracked in a living organism using the 3D real-time orbital tracking approach.

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OPERANDO STM OF CATALYTIC REACTIONS

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The concept of active sites is fundamental to heterogeneous catalysis. It is the idea that not the entire surface of a catalyst is active, but only certain elements which are different from the rest of the surface, e.g., by a special configuration of surface atoms at defects. However, for almost all reactions the exact nature of the active sites is unknown. The experimental problem is to get atomic scale information about the surface during a catalytic reaction, which usually takes place at a high pressure and at an elevated temperature.
By means of a scanning tunneling microscope (STM) that has specially been designed to work under reaction conditions it has been achieved to identify the active sites of the cobalt-catalyzed Fischer-Tropsch synthesis. In industry, the reaction is a large-scale process in which a mixture of CO and H2, so-called synthesis gas, reacts to give hydrocarbons for use as liquid fuels. The STM that was used for the experiments can be operated at pressures up to 1 bar and temperatures around 500 K, conditions that are sufficiently close to those applied in the industrial process. Using a single crystal cobalt sample as model catalyst, the formation of light hydrocarbons up to butane could be detected in the same apparatus, so that a catalytic turnover frequency could be determined. The STM data, taken on the same sample under the same conditions, showed that the surface displayed atomic steps. In a series of experiments the density of atomic steps could be varied by means of argon ion sputtering, and it turned out that the turnover frequency linearly scaled with the density of steps.
Atomic steps were in this way identified as the active sites. The role of the steps is probably to provide a particularly stable adsorption geometry for the CO molecules, in which the C atom binds to the lower edge of the step and the O atom to the upper edge. Starting from this geometry the cleavage of the C-O bond, most likely the rate-limiting step of the Fischer-Tropsch synthesis, is facilitated.

▪ **B. Böller, K. M. Durner, J. Wintterlin:** *The active sites of a working Fischer-Tropsch catalysts revealed by operando scanning tunnelling microscopy;* Nature Catalysis, 10.1038/s41929-019-0360-1 (2019).

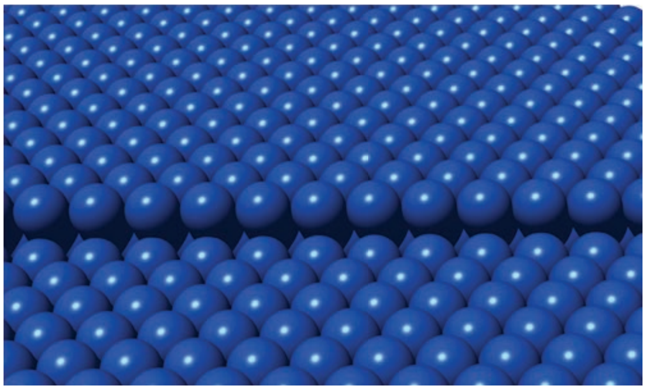

Fig. 1: Atomic model of a step on the Co(0001) surface. These defects have been identified as the active sites of the Fischer-Tropsch synthesis.

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SINGLE MOLECULE STUDIES ON OPTICAL ANTENNA SYSTEMS

Kristina Hübner, Johann Bohlen, Lennart Grabenhorst, Florian Selbach, Fernando Stefani, Jan Vogelsang, John Lupton, Guillermo Acuna, Tim Liedl, and Philip Tinnefeld
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Optical antennas are able to control light at the nanoscale and manipulate the photophysical properties of single photon emitters. To build optical antennas the group of Philip Tinnefeld uses DNA origami structures, which enable a nanometer positioning control of fluorescent dyes and plasmonic nanoparticles. The antenna's influence on emitters can be investigated on a single molecule level by different kind of measurements.

In a first approach the influence of an optical antenna on the excitation and emission angle of a single fluorescent dye is analysed. The combination of wide-field defocused imaging and polarization-resolved excitation measurements give the possibility to extract the emission and excitation angle, respectively. A correlation shows that the excitation and emission angle of a free rotating dye gets dominated and directed by the antenna. [1] A second effect studied together with the group of John Lupton from University of Regensburg is the fluorescence lifetime of a single fluorophore, which gets highly quenched by the optical antenna. To study this in more detail a setup with high temporal resolution is needed. The new introduced femtosecond double-excitation (FeDEx) photon correlation technique gives rise to measure fluorescence lifetimes not limited by the instrument response function (IRF) of the detector, but by the length of a laser pulse. This technique enables to measure the fluorescence lifetimes of the coupled dye nanoparticle systems down to 19 ps. [2] So far measurements were performed only on the level of one dye being present in the enhanced electric field near a plasmonic nanoparticle. To answer the question of the influence of a nanoparticle on a FRET (Förster resonance energy transfer) pair, a donor-acceptor system is positioned close to nanoparticles of different size. By the acceptor bleaching approach the FRET rate constant and efficiency are extracted based on the donor lifetime. It is shown that donor as well as acceptor experience the plasmon-assisted Purcell enhancement, but the effect on the FRET rate stays negligible, which in turn leads to a reduction of the transfer efficiency. [3]

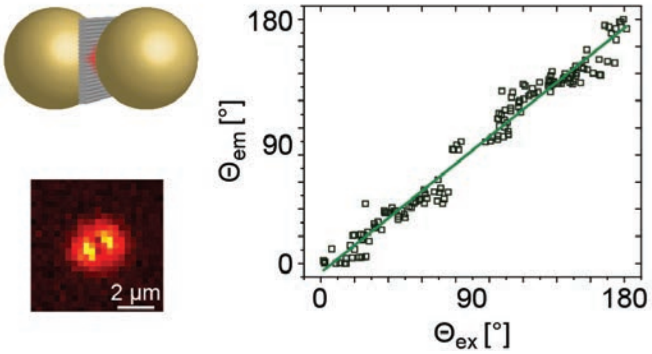

Fig. 1: A sketch of a DNA origami nanoantenna structure is shown in the upper left corner. The lower left image shows a defocused wide field image of the structure indicating a dipolar emission pattern. A correlation of the emission and excitation angle is plotted on the right side showing a strong correlation of both angles.

■ **[1] K. Hübner, M. Pilo-Pais, F. Selbach, T. Liedl, P. Tinnefeld, F. Stefani, G. Acuna:** *Directing single-molecule emission with DNA origami-assembled optical antennas;* Nano Letters DOI 10.1021/acs.nanolett.9b02886 (2019).

[2] J. Schedlbauer, P. Wilhelm, L. Grabenhorst, M.E. Federl, B. Lalkens, F. Hinderer, U. Scherf, S. Höger, P. Tinnefeld, S. Bange, J. Vogelsang, J.M. Lupton: *Ultrafast Single-Molecule Fluorescence Measured by Femtosecond Double-Pulse Excitation Photon Antibunching;* Nano Letters DOI 10.1021/acs.nanolett.9b04354 (2020).

[3] J. Bohlen, Á. Cuartero-González, E. Pibiri, D. Ruhlandt, A.I. Fernández-Domínguez, P. Tinnefeld, G.P. Acuna: *Plasmon-assisted Förster resonance energy transfer at the single-molecule level in the moderate quenching regime;* Nanoscale DOI 10.1039/C9NR01204D (2019).

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ULTRAFLEXIBLE NANOWIRE ARRAY FOR LABEL- AND DISTORTION-FREE CELLULAR FORCE TRACKING

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Mechanical forces between cells and the surrounding extracellular matrix play a crucial role for cellular functions in living organisms. The elucidation of cellular force generation is thus of fundamental interest to obtain further insights into the physics of life. Recently, a novel transducer for label-free cellular force tracking has been presented. Unlike other types of cellular force sensors, it avoids optical distortions which arise from the refractive index mismatch between the cells and the surrounding medium.
The device consists of an array of top-down nanostructured, ultraflexible nanowires. Its universal building block is an inverted conical semiconductor nanowire. The nanowire dimensions and thus its sensitivity are fully controlled by electron-beam lithography and plasma etching parameters. Typical nanowires feature a length of approx. 10 µm and head (foot) diameters of 800 nm (100 nm), which yields ultra-compliant spring constants in the range of 1 µN/nm or below. For nanowire separations exceeding 3 µm, the cells are found to penetrate into the array rather than spreading across the nanowire heads. This allows to perform microscopy on the nanowire heads while the cells deflecting the nanowires are confined within the array. The resulting separation between the optical path and the cells under investigation excludes optical distortions caused by cell-induced refraction, which can give rise to feigned displacements on the 100 nm scale. The undistorted nanowire displacements are converted into cellular forces via the nanowire spring constant. The resulting distortion-free cellular force transducer realizes a high-resolution and label-free biosenor based on optical microscopy. Its performance is demonstrated in a proof-of-principle experiment with living *Dictyostelium discoideum* cells migrating through the nanowire array. Cell-induced forces are probed with a resolution of 50 pN, while the most flexible nanowires promise to enter the 100 fN realm.

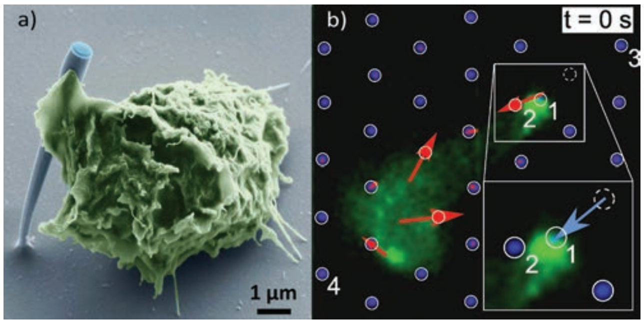

Fig. 1: Deflection of nanowires by migrating *D. discoideum* cell. (a) Scanning electron micrograph of a *D. discoideum* cell (green) immobilized during migration through a nanowire (blue) array with a period of 7 µm. (b) Overlays of the two simultaneously acquired optical images, showing the fluorescence of a Lim-GFP-labeled *D. discoideum cell* (green) and the optical reflection of the nanowire heads (blue). Nanowire deflections are visualized by arrows. The inset highlights a particularly strongly displaced nanowire which has been deflected by 3.7 µm.

- **P. Paulitschke, F. Keber, A. Lebedev, J. Stephan, H. Lorenz, S. Hasselmann, D. Heinrich, E. M. Weig:** *Ultra-flexible nanowire array for label- and distortion-free cellular force tracking;* Nano Letters 19 (4), 2207-2214 (2019), Cover Article.

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MECHANISTIC INSIGHTS INTO MICROSECOND TIMESCALE MOTION OF SOLID PROTEINS USING COMPLEMENTARY 15N AND 1H RELAXATION DISPERSION TECHNIQUES

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NMR relaxation dispersion methods provide a holistic way to observe microsecond timescale protein backbone motion both in solution and in the solid state. Different nuclei (1H and 15N) and different relaxation dispersion techniques (Bloch-McConnell and near-rotary-resonance) give complementary information about the amplitudes and timescales of the conformational dynamics and provide comprehensive insights into the mechanistic details of the structural rearrangements. In this paper, we exemplify the benefits of the combination of various solution- and solid-state relaxation dispersion methods on a microcrystalline protein (alpha-spectrin SH3 domain), for which we are able to identify and model the functionally relevant conformational rearrangements around the ligand recognition loop occurring on multiple microsecond timescales. The observed loop motions suggest that the SH3 domain exists in a binding-competent conformation in dynamic equilibrium with a sterically impaired ground state conformation both in solution and in crystalline form. This inherent plasticity between the interconverting macrostates is compatible with a conformational-preselection model and provides new insights into the recognition mechanisms of SH3 domains.

- **P. Rovó, C. A. Smith, D. Gauto, B. L. de Groot, P. Schanda, R. Linser:** *Mechanistic insights into microsecond timescale motion of solid proteins using complementary 15N and 1H relaxation dispersion techniques;* J. Am. Chem. Soc. doi: 10.1021/jacs.8b09258 (2019).

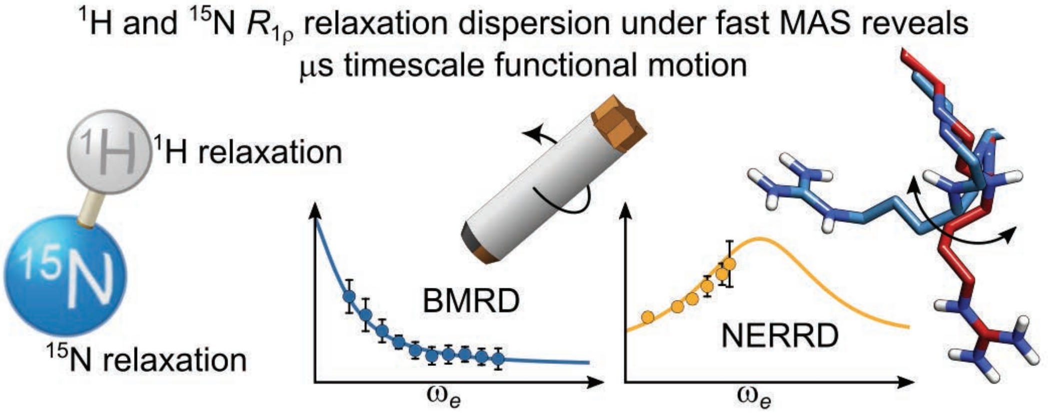

Fig. 1: The simultaneous measurement of both 1H and 15N relaxation dispersion at low field strength (BMRD regime) and at high field strength (NERRD regime) enables the holistic characterization of microsecond timescale protein backbone motion in the solid state.

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STUDYING INTERCHROMOPHORIC INTERACTIONS FOR SUPER RESOLUTION MICROSCOPY

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Small point light sources are crucial for characterizing a fluorescence microscope. The development of new small and bright point light sources did not keep up with the needs of the field of super resolution microscopy and biomolecular imaging. To this day, dye loaded polymer beads are used but exhibit substantial heterogeneity in size, brightness and shape. The group of Philip Tinnefeld used DNA origami structures as scaffold for ultra-bright point light sources. Dye molecules were arranged in a dense pixel array with high control of stoichiometry and dye-dye distance to find the highest labeling density that maintains a dye’s photophysics. Dye-dye distances were altered on the single base pair step and the dye-dye interactions were probed on the single molecule level. For small distances strong intensity and lifetime quenching is observed due to a combination of static and dynamic quenching. With increasing distance, we observe reduced quenching and dynamics in the DNA origami structure. At 3 nm distance the dyes are physically separated but energy transfer processes in the weak coupling regime still have a significant impact. The energy transfer between dyes can have both, beneficial or detrimental aspects for a point light source. Annihilation processes can lead to saturation at high excitation rates but it can also open new photophysical pathways for dark-state depopulation. This study fills a gap of studying the interactions of dyes relevant for dye arrangements in bright point light sources for super resolution microscopy. These findings will pave the way to create small, bright and homogeneous DNA origami nanobeads by preserving the photophysical properties of the dyes used.

- **T. Schröder, M.B. Scheible, F. Steiner, J. Vogelsang, P. Tinnefeld:** *Interchromophoric Interactions Determine the Maximum Brightness Density in DNA Origami Structures;* Nano Letters DOI 10.1021/acs.nanolett.8b04845 (2019).

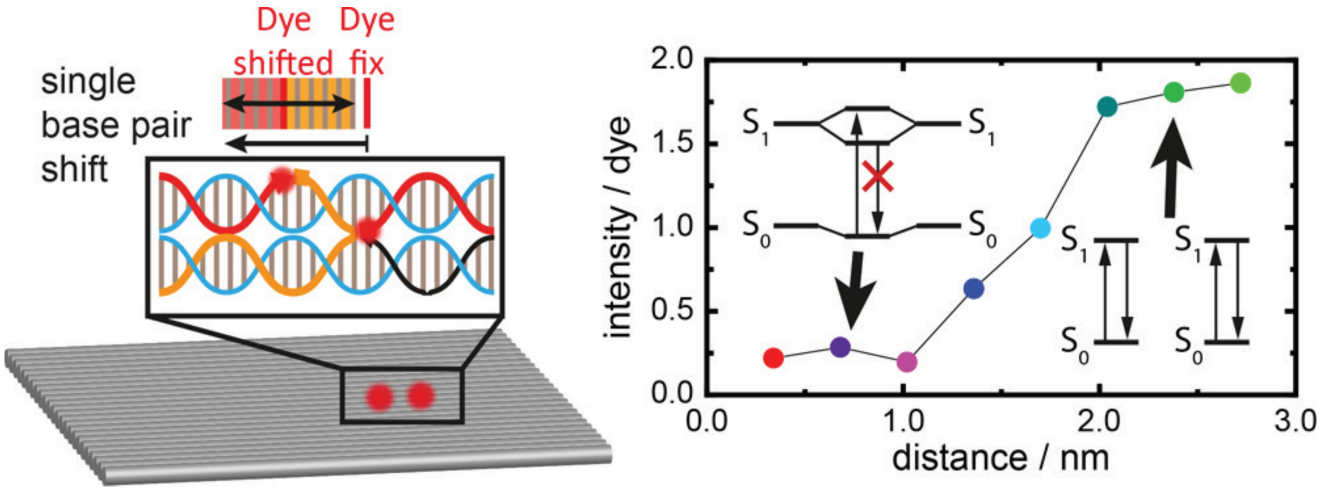

Fig. 1: *Left:* Model of the rectangular DNA origami structure labeled with two ATTO647N dyes for dye-dye interaction studies. *Right:* Average sample brightness vs. distance assuming that 1 base pair corresponds to 0.34 nm. Small distances show quenched fluorescence intensity due to H-type dimer formation. At 3 nm separation fluorescence intensity is fully recovered.

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COORDINATIVE BINDING OF POLYMERS TO METAL–ORGANIC FRAMEWORK NANOPARTICLES FOR CONTROL OF INTERACTIONS AT THE BIOINTERFACE

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Metal–organic framework nanoparticles (MOF NPs) are of growing interest in diagnostic and therapeutic applications, and due to their hybrid nature, they display enhanced properties compared to more established nanomaterials. The effective application of MOF NPs, however, is often hampered by limited control of their surface chemistry and understanding of their interactions at the biointerface. Using a surface coating approach, we found that coordinative polymer binding to Zr-fum NPs is a convenient way for peripheral surface functionalization. Different polymers with biomedical relevance were assessed for the ability to bind to the MOF surface. Carboxylic acid and amine containing polymers turned out to be potent surface coatings and a modulator replacement reaction was identified as the underlying mechanism. The strong binding of polycarboxylates was then used to shield the MOF surface with a double amphiphilic polyglutamate–polysarcosine block copolymer, which resulted in an exceptional high colloidal stability of the nanoparticles. The effect of polymer coating on interactions at the biointerface was tested with regard to cellular association and protein binding, which has, to the best of our knowledge, never been discussed in literature for functionalized MOF NPs. We conclude that the applied approach enables a high degree of chemical surface confinement, which could be used as a universal strategy for MOF NP functionalization. In this way, the physicochemical properties of MOF NPs could be tuned, which allows for control over their behavior in biological systems.

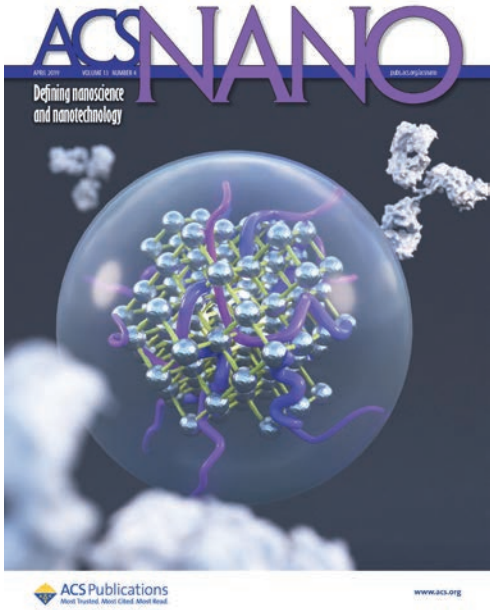

Fig. 1: Peripheral surface functionalization of metal–organic framework (MOF) nanoparticles by coordinative binding of polymers tunes the physicochemical properties and interactions at the biointerface: a hydrophilic block copolymer with a separate MOF binding segment creates a steric shield around the nanoparticles which avoids aggregation and interaction with immunoglobulins.

- **A. Zimpel, N. Danaf, B. Steinborn, J. Kuhn, M. Höhn, T. Bauer, P. Hirschle, W. Schrimpf, H. Engelke, E. Wagner, M. Barz, D.C. Lamb, U. Lächelt, S. Wuttke:** *Coordinative Binding of Polymers to Metal–Organic Framework Nanoparticles for Control of Interactions at the Biointerface;* ACS Nano, doi 10.1021/acsnano.8b06287 (2019).

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COLLECTIVE DYNAMICS OF STRAIN-COUPLED NANOMECHANICAL PILLAR RESONATORS

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Semiconductur nano- and micropillars represent a promising platform for hybrid nanodevices. Their ability to couple to a broad variety of nanomechanical, acoustic, charge, spin, excitonic, polaritonic, or electromagnetic excitations is utilized in fields as diverse as force sensing or optoelectronics. In order to fully exploit the potential of these versatile systems e.g. for metamaterials, synchronization or topologically protected devices an intrinsic coupling mechanism between individual pillars needs to be established. This can be accomplished by taking advantage of the strain field induced by the flexural modes of the pillars. In a recent experiment, the strain-induced coupling between two adjacent nanomechanical pillar resonators has been demonstrated for the first time.
The system under investigation is a pair of top-down fabricated semiconductor nanopillars, with typical lengths of 7 µm, head (foot) diameters of approx. 1 µm (600 nm) and a separation of approx. 1 µm. The four fundemental flexural modes of the pillar pair are explored by two complementary techniques: Scanning electron microscopy under mechanical driving reveals clear signatures of mode hybridization. Optical interferometry allows to probe the mode's response to the drive frequency under laser-induced thermal eigenfrequency tuning. For sufficiently small nanopillar separation, the formation of an avoided level crossing is observed, demonstrating a nanopillar interaction in the strong coupling regime. This may be an important asset in overcoming the fabricational disorder-induced detuning of multiple nanopillars. The described coupling mechanism is readily scalable to larger arrays, enabling hybrid nanomechanical resonator networks for the investigation of a broad range of collective dynamical phenomena.

- **J. Doster, S. Hoenl, H. Lorenz, P. Paulitschke, E. M. Weig:** *Collective dynamics of strain-coupled nanomechanical pillar resonators;* Nature Communications 10, 5246 (2019).

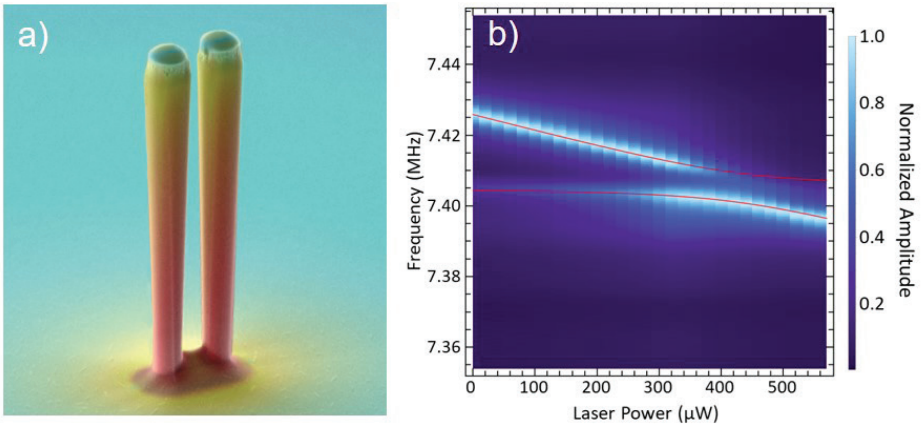

Fig. 1: Strain-induced coupling between two nanopillar resonators. (a) Overlay of a scanning electron micrograph of the nanopillar pair and the simulated strain distribution of one of the system's vibrational eigenmodes. (b) Avoided level crossing between a flexural mode of the left and the right nanopillar. The laser power of the detection laser is employed to thermally tune the flexural modes of one of the nanopillars.

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KINETICS AND THERMODYNAMICS OF ON-SURFACE COUPLING REACTIONS

Massimo Fritton, **Wolfgang M. Heckl,** and **Markus Lackinger**

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Coupling of molecules on solid surfaces affords unique low-dimensional covalent organic nanostructures. Yet, on-surface synthesis largely builds on empiricism, while for the improvement of structural quality through a systematic optimization of reaction parameters a fundamental understanding of the surface chemistry is needed. For most relevant reactions it is not even clear whether decisive reaction steps are kinetically or thermodynamically controlled. To shed more light on this crucial aspect, a comparative study was carried out on Ag(111) vs. Au(111) surfaces. The used threefold symmetric brominated monomer couples covalently on both surfaces, but the network quality can vary substantially. Often samples are just characterized by Scanning Probe Microscopy. While this approach unveils structural details, it lacks the chemical and temporal resolution required for elucidating the surface chemistry. To this end we employed Temperature-Programmed X-ray Photoelectron Spectroscopy (TP-XPS), where samples are continuously monitored by XPS while being heated with a linear temperature ramp. Superior chemical and temporal resolution is achieved with synchrotron radiation.

By means of TP-XPS we studied both the initial debromination that activates covalent bond formation and the conversion of the organometallic intermediates on Ag(111) into their covalent final products. Striking differences were found for the debromination: it occurs rapidly on Ag(111), whereas on Au(111) the debromination proceeds unexpectedly gradual. The results on Ag(111) can be modelled by first order reaction kinetics, whereas on Au(111) the experimental data could only be reproduced by a thermodynamic model with input from density functional theory. These findings indicate and substantiate a vitally important role of reaction parameters for the structural quality of the products. Accordingly, the optimization of preparation protocols bears great potential for improving on-surface synthesis.

■ **M. Fritton, D.A. Duncan, P.S. Deimel, A. Rastgoo-Lahrood, F. Allegretti, J.V. Barth, W.M. Heckl, J. Björk, and M. Lackinger:** *The role of kinetics vs. thermodynamics in surface-assisted Ullmann coupling on gold and silver surface;* J. Am. Chem. Soc., 10.1021/jacs.8b11473 (2019).

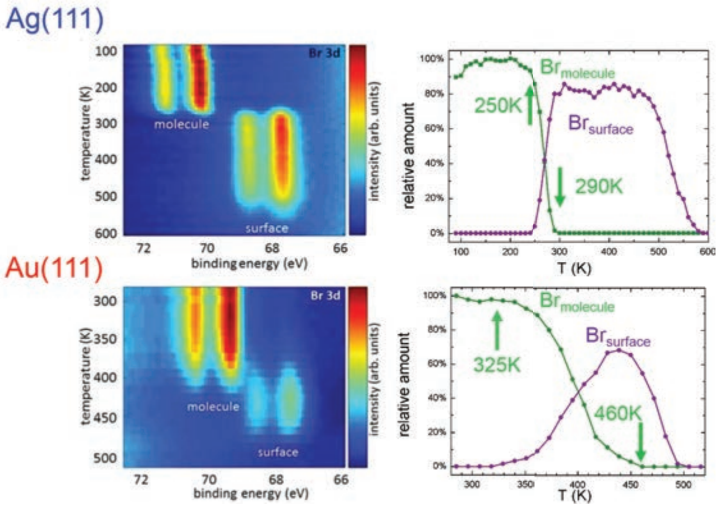

Fig. 1: TP-XPS data acquired on Ag(111) (upper row) vs. Au(111) (lower row). The surface-mediated debromination of 1,3,5-tris(4′-bromophenyl) benzene was tracked by measuring Br 3d core levels. The doublet at higher binding energies originates from molecule-bound bromine, while surface-bound bromine gives rise to a doublet at lower binding energies. The graphs on the right hand side depict the relative intensities of molecule-bound (green curves) vs. surface-bound (violet curves) bromine as obtained from fitting the individual spectra. Temperatures for both onset and completion of debromination are indicated.

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SUPRAMOLECULAR ASSEMBLY OF AMINOETHYLENE-LIPOPEPTIDE PMO CONJUGATES INTO RNA SPLICE-SWITCHING NANOMICELLES

Jasmin Kuhn, P.M. Klein, Nader Al Danaf, Joel Z. Nordin, Sören Reinhard, Dominik M. Loy, Miriam Höhn, Samid El Andaloussi, **Don C. Lamb, Ernst Wagner**, Yoshitsugo Aoki, Taavi Lehto, and **Ulrich Lächelt**

- www.cup.lmu.de/pc/lamb
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- www.cup.lmu.de/pb/aks/ewagner/members/dr-ulrich-laechelt

Phosphorodiamidate morpholino oligomers (PMOs) are oligonucleotide analogs that can be used for therapeutic modulation of pre-mRNA splicing. Similar to other classes of nucleic acid-based therapeutics, PMOs require delivery systems for efficient transport to the intracellular target sites. In the research project a novel highly potent molecular transporter for PMOs was developed. It consists of an artificial lipopeptide covalently conjugated to the PMO and self-assembles into nanomicelles with strongly enhanced cellular uptake. The work shows that mRNA splicing can efficiently be modified in different tumor cells as well as myotubes derived from a Duchenne muscular dystrophy (DMD) mouse model. DMD is a severe disease which generally begins during childhood with extensive muscle loss. Splice-switching represents a promising option for treatment of the fatal genetic disease. The international, multi-collaborative work resulted in the identification of highly potent aminoethylene-lipopeptides for the generation of PMO-therapeutics with a favorable activity/toxicity profile

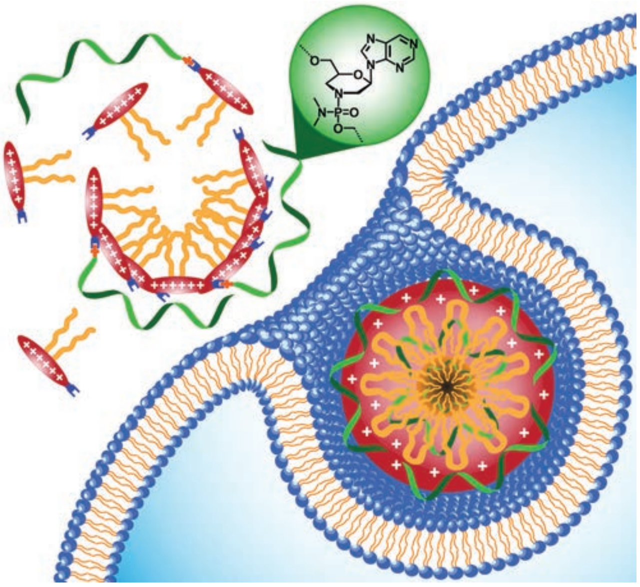

Fig. 1: Schematic illustration of the nanomicelle formation from splice-switching PMO conjugates.

- **J. Kuhn, P.M. Klein, N. Al Danaf, J.Z. Nordin, S. Reinhard, D.M. Loy, M. Höhn, S. El Andaloussi, D.C. Lamb, E. Wagner, Y. Aoki, T. Lehto, U. Lächelt:** *Supramolecular Assembly of Aminoethylene-Lipopeptide PMO Conjugates into RNA Splice-Switching Nanomicelles;* Adv. Funct. Mater., doi 10.1002/adfm.201906432 (2019).

27

SUSTAINED SOLAR H_2 EVOLUTION FROM A THIAZOLO[5,4-D]THIAZOLE-BRIDGED COVALENT ORGANIC FRAMEWORK AND NICKEL-THIOLATE CLUSTER IN WATER

Bishnu P. Biswal, Hugo A. Vignolo-González, Tanmay Banerjee, Lars Grunenberg, Gökcen Savasci, Kerstin Gottschling, Jürgen Nuss, **Christian Ochsenfeld,** and **Bettina V. Lotsch**

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The conversion and storage of solar energy in the form of chemical bonds in "solar fuels" such as H_2 through light-driven water reduction has evolved into a key technology over the last decade, driven by fast depletion of fossil energy sources and rapid global climate change. The research on solar H_2 evolution from water utilizing fully organic networks such as covalent organic frameworks (COFs) as heterogeneous photosensitizers has been gathering significant momentum over the past years, as COFs offer a unique set of properties, including crystallinity and ordered porosity, controllable light harvesting and tunable photophysical properties, all within a molecularly precise, yet robust backbone.

Prior to this work, COFs had been utilized as photoabsorbers for photocatalytic H_2 evolution mostly in conjunction with metallic platinum nanoparticles as the co-catalyst (a rare and expensive metal), which appears to be the bottleneck towards scalable, economical solar H_2 production. In addition, the use of nanoparticulate Pt co-catalysts precludes detailed insights into the nature of the catalytic sites and the intricacies of the photocatalytic cycle.

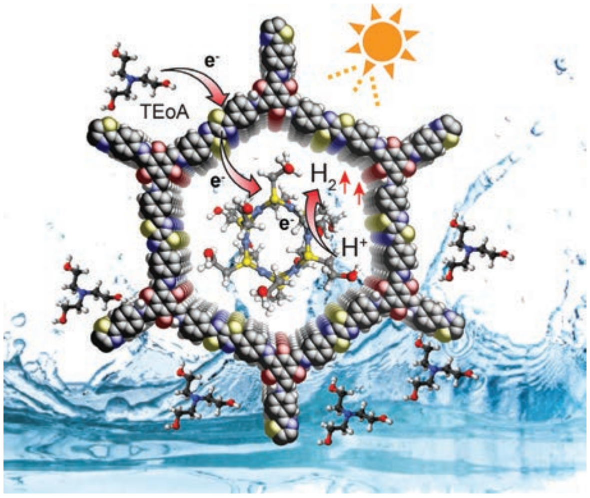

Fig. 1: General scheme of the proposed pathway for photocatalytic H_2 evolution reaction with TpDTz COF and NiME cluster co-catalyst in water (color code: grey; C, red; O, yellow; S, blue; N and light pink/white; H).

This work demonstrates the first COF single-site photocatalyst that is photochemically stable over tens of hours and operates with a noble-metal free, hexameric Ni-based co-catalyst in water and triethanolamine as the sacrificial electron donor. The observed high H_2 evolution rate and long-term operation of this hybrid system in water surpasses that of many state-of-the-art organic dyes, carbon nitride and COF-sensitized photocatalytic water reduction systems. In addition, the novel flow reactor design used in this study enabled the non-invasive and direct monitoring of the H_2 evolution rate with high accuracy, providing in-depth insights into the photocatalytic mechanism and the complex kinetics of the reaction system. Microkinetic modeling suggests that an outer-sphere electron transfer from the photoabsorber to the catalyst is the rate-limiting step, thus spotlighting the importance of the rational design of the COF–co-catalyst interface. Quantum-chemical theoretical calculations were instrumental at providing an atomistic understanding of the interaction between COF and co-catalyst as well as the feasibility of electron transfer processes, thus enabling detailed mechanistic insights to establish structure-property-activity relationships in this system.

In perspective, this study contributes to the rational design of robust, noble-metal free and efficient single-site COF–molecular co-catalyst hybrid systems for the sustained generation of solar fuels from water.

- **B. P. Biswal, H. A. Vignolo-González, T. Banerjee, L. Grunenberg, G. Savasci, K. Gottschling, J. Nuss, C. Ochsenfeld, B. V. Lotsch:** *Sustained Solar H2 Evolution from a Thiazolo[5,4-d]thiazole-Bridged Covalent Organic Framework and Nickel-Thiolate Cluster in Water;* J. Am. Chem. Soc. DOI: 10.1021/jacs.9b03243 (2019); (Published as 'Supplementary Cover Page' of JACS).

28

COORDINATIVE METAL-DRUG NANOPHARMACEUTICALS

Benjamin Steinborn, Patrick Hirschle, Miriam Höhn, T. Bauer, M. Barz, **Stefan Wuttke, Ernst Wagner**, and **Ulrich Lächelt**

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Selected drug molecules with Lewis base functions can be assembled into coordinative nanoparticles (NPs) by linking them with suitable metal ions. Such nanomaterials exhibit a high material economy due to high drug contents and minor amounts of inactive additives. The antifolate pemetrexed (PMX) which is used for the treatment of lung cancers contains two carboxy functions that are able to undergo coordinative binding of metal ions. This study presents the development of a multilayer PMX NP system where each layer serves a distinct purpose. The metal-drug NP core is assembled in a bottom-up approach by coordinative interactions between zirconium (IV) ions and PMX molecules. Since the NP core is generated from drug molecules as essential units, it features a very high drug content of almost 80%. The NP core is stabilized against serum with a shell of a polymerized oligoamine-modified trimethoxysilane derivative (TMSP). As external layer, a polyglutamate-block-polysarcosine-N3 (pGlu-b-pSar) coating mediates efficient colloidal stabilization and enables introduction of targeting functionalities by click chemistry. Attaching folate or transferrin ligands to the polymer layer enhances NP uptake into target receptor positive KB and L1210 cells. This study illustrates the development and characterization of metal-drug coordination NPs with high drug content and variable external functionalizations.

- **B. Steinborn, P. Hirschle, M. Höhn, T. Bauer, M. Barz, S. Wuttke, E. Wagner, U. Lächelt:** *Core-Shell Functionalized Zirconium-Pemetrexed Coordination Nanoparticles as Carriers with a High Drug Content;* Adv. Therap., doi 10.1002/adtp.201900120 (2019).

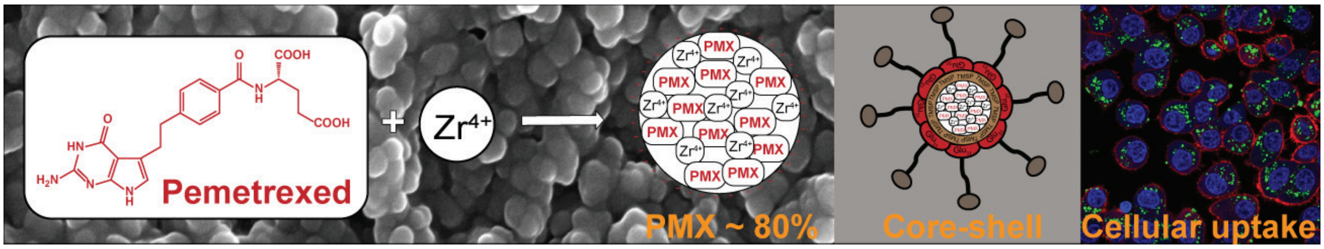

Fig. 1: Illustration of the multi-layer chemotherapeutic nanoparticle based on a coordinative zirconium-pemetrexed core with a drug content of almost 80 %. Sequential functionalization with an oligoamine-modified silica-reagent and a targeted polyglutamate-polysarcosine block-copolymer as the outermost layer mediates shielding, increases colloidal stability and enhances nanoparticle uptake into cancer cells via target receptors.

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INSIGHTS INTO CHEMISTRY THROUGH THE COMPUTATION OF FREE ENERGY HOT-SPOTS

Johannes C. B. Dietschreit, Laurens D. M. Peters, Jörg Kussmann, and **Christian Ochsenfeld**
■ www.cup.uni-muenchen.de/pc/ochsenfeld/

While free energy changes can be computed using a variety of methods, the interpretation of free energy differences is in most cases not straightforward, because it is not possible to separate out and localize contributions from different atoms or residues, inhibiting insights into the underlying effects. Therefore, we have developed a new method that allows for a detailed interpretation of free energy changes [1,2]. Our method calculates the vibrational part of the free energy from the vibrational density of states function and locates the changes in the potential energy surface. These so-called hot-spots indicate the locations causing the overall free energy to change. Here, our ansatz is applicable to any level of theory employed for generating the dynamics simulation.

As first example in applying our new partitioning method, we investigated the reversible binding of an inhibitor to a protein with molecular mechanics simulations. We selected the bromodomain, which is involved in the recognition of acetylated lysine residues. Our method indicates – in line with chemical intuition - that upon binding the inhibitor, the protein potential energy surface is modified leading to conformational changes in the protein that cause the binding site to tighten around the inhibitor molecule (see Fig. 1). Our method allows to locate areas of lower and higher flexibility which can be important when devising new inhibitors.

As a second example we investigated the well-known anomeric effect that occurs in heterocycles such as sugars. It leads to the stabilization of otherwise sterically disfavoured configurations, e.g., an unexpected stabilisation of α-glucose with respect to β-glucose. We simulated several configurations and modifications of glucose at the ab-initio level and were able to single out the atoms influencing the process.

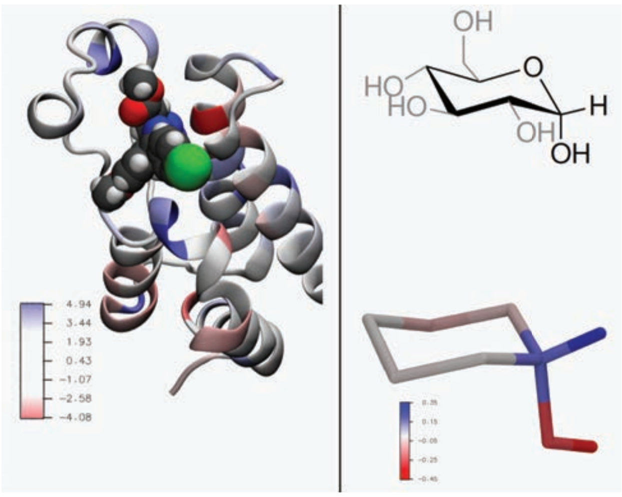

Fig. 1: The left half shows the vibrational free energy change within the bromodomain upon inhibitor binding. The colour scale is shown in left bottom corner. Blue indicates a gain in free energy (tightening), red a loss (loosening). On the right, we show the centre skeleton of glucose (structure shown at the top) and the atoms involved in the anomeric effect carrying a free energy change clearly different from zero.

In this way, our new approach allows for general applicability at any level of the potential energy surface and to interpret free energy calculations for gaining novel insights into complex processes.

■ [1] **J. C. B. Dietschreit, L. D. M. Peters, J. Kussmann, C. Ochsenfeld:** *Identifying free energy hot-spots in molecular transformations;* J. Phys. Chem. A, 10.1021/acs.jpca.8b12309 (2019).

[2] **L. D. M. Peters, J. C. B. Dietschreit, J. Kussmann, C. Ochsenfeld:** *Calculating free energies from the vibrational density of states function: validation and critical assessment*; J. Chem. Phys., 10.1063/1.5079643 (2019).

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HEMITHIOINDIGOS FOR CELLULAR PHOTOPHARMACOLOGY

Alexander Sailer, Franziska Ermer, Yvonne Kraus, Ferdinand Lutter, Carsten Donau, Maximilian Bremerich, Julia Ahlfeld, and **Oliver Thorn-Seshold**

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Druglike small molecules with photoswitchable bioactivity — photopharmaceuticals — allow biophysical studies with exquisitely precise and reversible, spatial and temporal control over critical biological systems that are inaccessible to genetic manipulation. However, the photoresponsive pharmacophores disclosed have been almost exclusively azobenzenes, which has limited the structural and substituent scope of photopharmacology. More detrimentally, for azobenzene reagents, it is not researchers' needs for adapted experimental tools, but rather protein binding site sterics, that typically force whether the trans (dark) or cis (lit) isomer is the more bioactive. To overcome this problem we have rationally designed the first hemithioindigo-based pharmacophores enabling photoswitchable control over endogenous biological activity in cellulo, and used them to optically control microtubule depolymerisation and cell death in unmodified mammalian cells. We show that the symmetry properties of hemithioindigos allow a priori design of either Z- or E- (dark- or lit)-toxic antimitotics, whereas the corresponding azobenzenes are exclusively lit-toxic. We thus demonstrate that hemithioindigos enable an important expansion of the substituent and design scope of photopharmacological interventions for biological systems.

■ **A. Sailer, F. Ermer, Y. Kraus, F. Lutter, C. Donau, M. Bremerich, J. Ahlfeld, O. Thorn-Seshold:** *Hemithioindigos for cellular photopharmacology: desymmetrised molecular switch scaffolds enabling design control over the isomer-dependency of potent antimitotic bioactivity;* ChemBioChem, doi 10.1002/cbic.201800752 (2019) *(Highlighted in the ChemBioTalents collection and in SynFacts).*

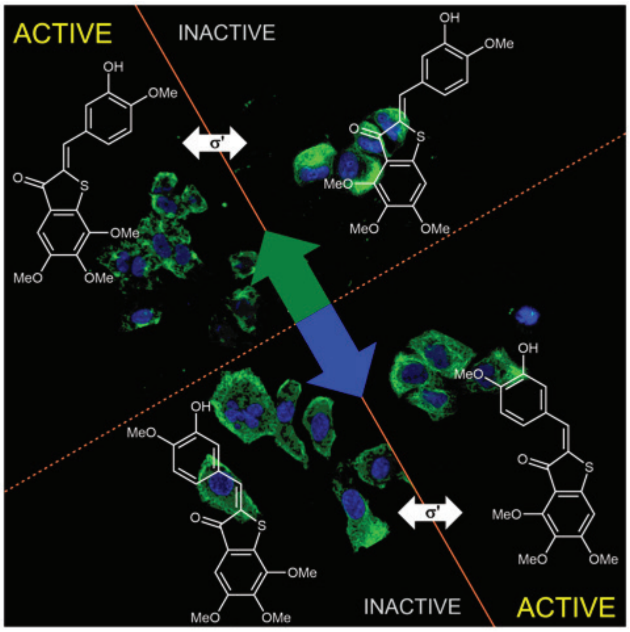

Fig. 1: Permuting substituents around the hemithioindigo scaffold swaps between Z- and E-binding structures. Hemithioindigo designs thus allow rational control over which photoisomer is the protein-binding form, rather than this form being set by protein sterics.

31

FORCES BETWEEN MOLECULES AND MOLECULAR COMPLEXES CHARACTERIZED BY MOLECULAR DYNAMICS SIMULATIONS AND SINGLE-MOLECULE FORCE SPECTROSCOPY

Ellis Durner, Constantin Schoeler, Klara H. Malinowska, Michael A. Nash, Res Jöhr, Magnus S. Bauer, Fabian Baumann, Leonard C. Schendel, Carleen Kluger, Markus A. Jobst, Lukas F. Milles, Diana A. Pippig, and **Hermann E. Gaub**
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Mechanobiology emerges at the crossroads of medicine, biology, biophysics and engineering and describes how the responses of proteins, cells, tissues and organs to mechanical cues contribute to development, differentiation, physiology and disease. To quantify how biological systems sense, transduce, respond and apply mechanical signals atomic force microscopy (AFM) is used to discover morphological and mechanical properties of biological systems.

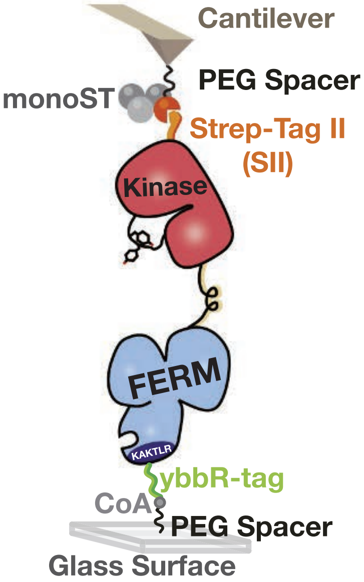

Fig.1: Mimicking the attachment of focal adhesion kinase in cells for the AFM force spectroscopy assay. The scheme illustrates the kinase on a PEG functionalized glass surface and monoST on the cantilever. The ybbr-tag ensures site-specific covalent attachment to the surface via an Sfp-catalyzed reaction with CoA connected to a PEG spacer. At the C-terminus, equipped with an SII reversible tethering to monoST on the cantilever is enabled.

The focal adhesion kinase localized in focal adhesion complexes formed at the cytoplasmic side of cell attachment was investigated (Fig.1). The experimental and computational approaches demonstrate how mechanical forces can induce conformational changes in Focal adhesion kinase that regulate cell adhesion, migration, and survival (M.S. Bauer *et al.*).

Accordingly the influence of the X-module on the force of the X-module-Dockerin interaction with Cohesin - important for the bacterium *Ruminococcus faciens* when dissecting cellulose from wood - was also studied by AFM force spectroscopy in concert with molecular dynamics simulations. The force propagation through the entire molecular complex (Fig.2) was understood on the level of individual atoms (R.C. Bernardi *et al.*).

The light-switchable fluorescent protein Dronpa can bind or release its binding partner dependent on the wavelength of incident light (Fig. 3). By AFM single molecule force spectroscopy Dronpa was characterized to even switch against external forces and thus might be utilized as an extension of the biomechanical toolbox to optically induce mechanical cues inside living cells (R. Jöhr *et al.*).

■ **R.C. Bernardi, E. Durner, C. Schoeler, K. H. Malinowska, B. G. Carvalho, E. A. Bayer, Z. Luthey-Schulten, H. E. Gaub, M. A. Nash:** *Mechanisms of Nanonewton Mechanostability in a Protein Complex Revealed by Molecular Dynamics Simulations and Single-Molecule Force Spectroscopy;* JACS, https://doi.org/10.1021/jacs.9b06776 (2019).

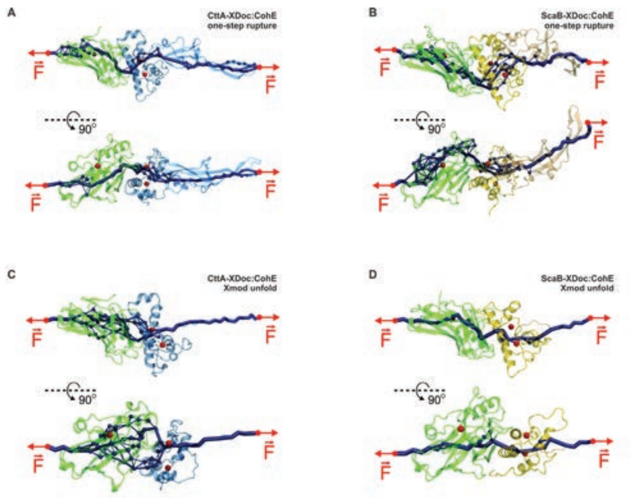

Fig.2: Evolution of force propagation pathways. Force propagation pathways were calculated from correlation-based network analysis carried out using SMD trajectories. For a one-step rupture of the complex CttA-XDoc:CohE force-propagation routes nonparallel to the pulling axis are observed near the Dockerin-Cohesin interface. Thicker tubes correspond to higher likelihood of force propagating through a path. The observed changes in force direction, present mostly as sharp turns in force propagation routes particularly near the interface, suggest that complexes formed by Cohesin and Dockerin achieve mechanostability by directing externally applied forces normal to the pulling axis because of the the X-module. Consequently, more force is required to achieve a given separation along the pulling axis.

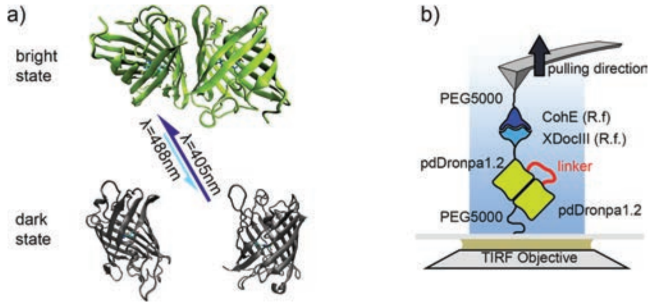

Fig.3: (a) Crystal structure of the fluorescent and dark state of Dronpa (bright and dark state). The bright state can be switched to the dark one by intense irradiation with blue light (λ = 488 nm). The back-switching is triggered by light at 405 nm. (b) Scheme of the experimental setup used for AFM-based SMFS.

M. S. Bauer, F. Baumann, C. Daday, P. Redondo, E. Durner, M. Andreas Jobst, L. F. Milles, D. Mercadante, D. A. Pippig, H. E. Gaub, F. Gräter, and D. Lietha: *Structural and mechanistic insights into mechanoactivation of focal adhesion kinase;* PNAS, https://doi.org/10.1073/pnas.1820567116 (2019).

R. Jöhr, M. S. Bauer, L. C. Schendel, C. Kluger, and H. E. Gaub: *Dronpa: A Light-Switchable Fluorescent Protein for Opto-Biomechanics;* Nano Lett, DOI: 10.1021/acs.nanolett.9b00639 (2019).

M. Krieg, G. Fläschner, D. Alsteens, B. M. Gaub, W. H. Roos, G. J. L. Wuite, H. E. Gaub, C.Gerber, Y. F. Dufrêne, and D. J. Müller: *Atomic force microscopy- based mechanobiology;* Nature Reviews Physics DOI: https://doi.org/10.1038/s42254-018-0001-7 (2019).

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MEASURING THE MULTIMERIZATION OF VON WILLEBRAND FACTOR AND ITS MECHANICAL STABILITY AT LOW FORCES MONITORING THE EARLY STEPS IN THE FORMATION OF BLOOD CLOTS

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Von Willebrand factor (VWF) is a shear force sensitive molecule in the blood stream that initiates the blood-clotting cascade. VWF circulates under normal conditions as a multimer in a compact globular form. At increased shear forces in the bloodstream -owing to injury of the vasculature- VWF elongates up to several micro meters and exposes binding sites to blood platelets and to collagen. Binding of VWF to platelets in turn triggers a reaction cascade that leads to clotting and sealing the wound. Mutations in VWF that impair multimerization can lead to subtype 2A of the bleeding disorder von Willebrand Disease. Here atomic force microscopy (AFM) imaging was provedn as a new method to determine the size distribution of VWF variants by direct visualization at the single-molecule level . Compared to common electrophoretic multimer analysis AFM resolved and quantified multimerization defects of pathologic VWF mutants (A. Löf, G.König *et al.*). For mimicking shear forces of the bloodstream, so far VWF was tugged between the AFM tip and a glass-substrate to observe stretching under the applied force. In a new magnetic tweezer (MT) approach a protein is attached between a tiny magnetic bead and the fluid cell substrate. Inducing an external magnetic field to hundreds of beads in parallel results in a vertical displacement of each bead, reporting the extension of the attached protein even for several days. Analysis of the stretching of VWF dimers with MT showed that a region of the VWF called the "stem" opens up under an applied force of 1 pN. In this region the subunits of the dimer are pulled apart like the two halves of a zipper. This new approach provides a detailed picture of the forces and the changes in extension involved in unfolding VWF (A. Löf, P. U.Walker *et al.*). Future applications of the method will not only contribute to a better understanding of the mode of action of VWF and of the role of clinically relevant mutations but also to many other mechano-sensitive molecules.

- **A. Löf, G. König, S. Schneppenheim, R. Schneppenheim, M. Benoit, U. Budde, J. P. Müller, and M. A. Brehm:** *Advancing multimer analysis of von Willebrand factor by single-molecule AFM imaging*; PLoS ONE, DOI http://dx.plos.org/10.1371/journal.pone.0210963 (2019)

A. Löf, P. U. Walker, S. M. Sedlak, S. Gruber, T. Obser, Maria A. Brehm, M. Benoit, and J. Lipfert: *Multiplexed protein force spectroscopy reveals equilibrium protein folding dynamics and the low-force response of von Willebrand factor;* PNAS, https://doi.org/10.1073/pnas.1901794116 (2019)

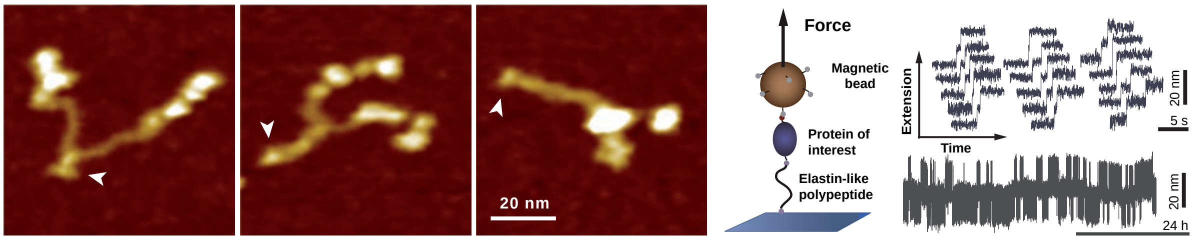

Fig. 1: AFM images of VWF dimers with an open, partly closed and fully closed "stem" (left). Highly parallel protein force spectroscopy with magnetic tweezers at low forces over several days (right).

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IMPORTANCE OF THE BIOFILM MATRIX FOR THE EROSION STABILITY OF BACILLUS SUBTILIS NCIB 3610 BIOFILMS

Merlin Klotz, Martin Kretschmer, Alexandra Goetz, Simone Ezendam, **Oliver Lieleg** and **Madeleine Opitz**

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The formation of biofilms leads to a competitive advantage of the bacterial biofilm forming community. Bacteria embedded within the biofilm are protected against antibiotics and other chemicals, and the structural rigidity provided by the biofilm matrix enables the bacterial community to withstand high shear forces or other mechanical stresses. In this study the authors combine different biophysical techniques to investigate how specific components of the biofilm matrix contribute to the erosion stability of biofilms formed by the bacterium *Bacillus subtilis* NCIB 3610. The authors demonstrate that the erosion stability of the biofilm decreases in the absence of the biofilm matrix and is correlated to changes in the hydrophobic surface properties of the biofilm as well as the biofilm stiffness. Furthermore, the authors investigate how the presence of metal ions or antibiotics influences the erosion stability of B. subtilis NCIB 3610.

- **M. Klotz, M. Kretschmer, A. Goetz, S. Ezendam, O. Lieleg and M. Opitz:** *Importance of the biofilm matrix for the erosion stability of Bacillus subtilis NCIB 3610 biofilms;* RSC Advances, doi:10.1039/c9ra01955c (2019).

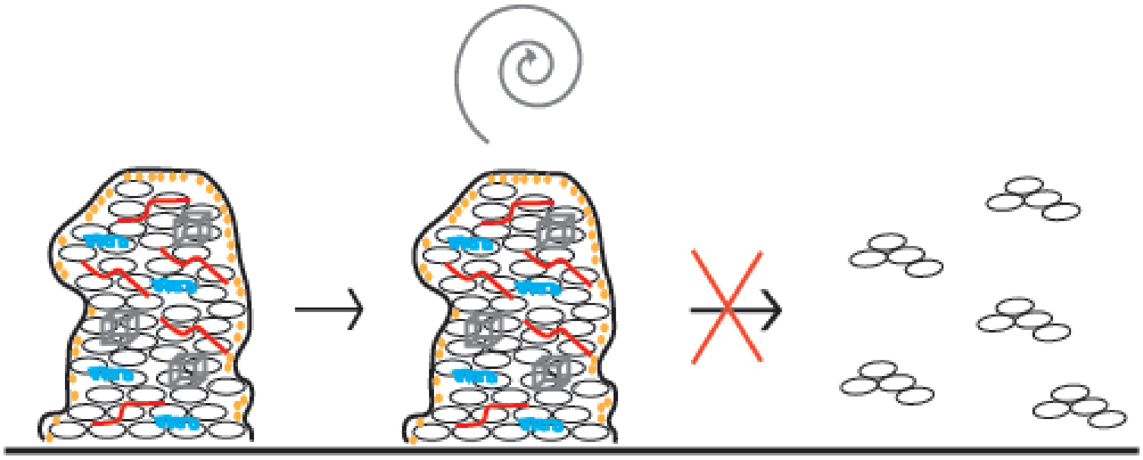

Fig. 1: The biofilm matrix protects the bacterial cells within the biofilm from erosion and destruction into smaller pieces. In the figure the different matrix components are indicated by grey (sugars), blue (fibrils) or red (fibers) symbols. Yellow dots indicate a hydrophobic protection protein layer present in *B. subtilis* NCIB 3610 biofilms. The grey spiral indicates the erosion process.

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ENGINEERING AN ORCHESTRATED RELEASE AVALANCHE FROM HYDROGELS USING DNA-NANOTECHNOLOGY

Ceren Kimna and **Oliver Lieleg**
■ www.mw.tum.de/en/bme

Most medical therapies require repeated, sequential administration of therapeutic agents in well-defined intervals and over extended time windows. Typically, the patient is in charge of applying the individual drug doses, and insufficient patient compliance reduces the efficiency of the treatment. Therefore, the development of a smart delivery mechanism releasing therapeutic agents in a pre-defined, time-controlled fashion would be beneficial for many medical treatments. We devised a DNA-mediated release cascade which allows for precisely controlling the sequential delivery of several different nanoparticles. By using complementary DNA sequences, nanoparticle aggregates can be created, embedded into distinct layers of a hydrogel and released by triggering aggregate dispersal. This mechanism is compatible with physiological conditions as the release cascade is initiated by exposing the nanoparticle-loaded gel to physiological salt concentrations. Moreover, the reservoir hydrogel can be enriched with biopolymers to receive charge-selective release properties towards small molecules - without interfering with the DNA-based release cascade. Owing to the excellent reproducibility, precision and effectiveness of the presented mechanism, a similar DNA-mediated release avalanche may lead to the development of autonomous and robust delivery systems, which minimize the possibility of pharmaceutical therapy failure due to patient non-compliance.

■ **C. Kimna and O. Lieleg:** *Engineering an orchestrated release avalanche from hydrogels using DNA-nanotechnology;* Journal of Controlled Release 304, 19-28 (2019).

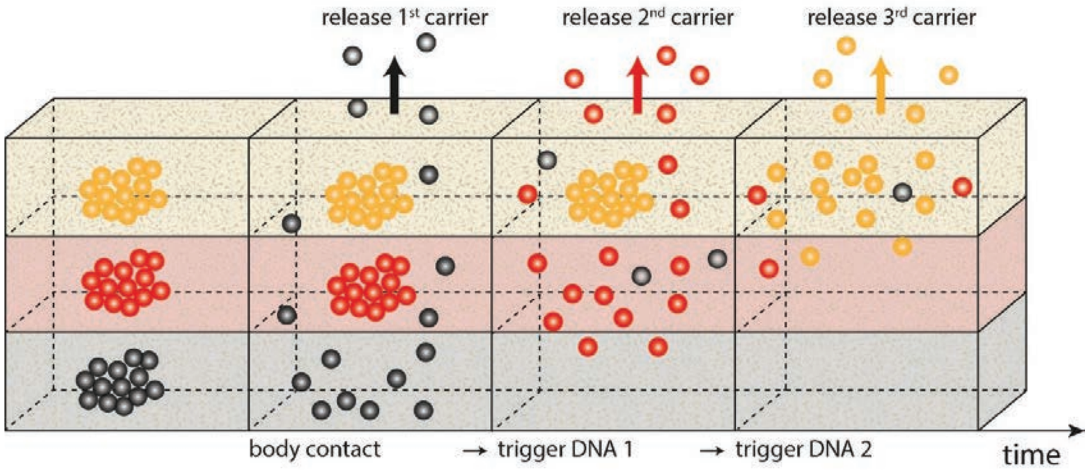

Fig. 1: A simplified schematic explaining the working principle of our approach. Once the nanoparticle-loaded hydrogel is brought into contact with a saline solution, the release avalanche is initiated from bottom to top. DNA strands released from the nanoparticle clusters located in the bottom layer serve as 'keys' which trigger the disassembly of nanoparticle clusters in the middle layer, which in turn liberate a 3rd nanoparticle species with the help of another released DNA sequence.

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